

9-Bromoanthracene

Other names:	9-Anthracenyl bromide anthracene, 9-bromo-
Inchi:	InChI=1S/C14H9Br/c15-14-12-7-3-1-5-10(12)9-11-6-2-4-8-13(11)14/h1-9H
InchiKey:	ZIRVQSRSPDUEOJ-UHFFFAOYSA-N
Formula:	C14H9Br
SMILES:	BrC1c2ccccc2cc2ccccc12
Mol. weight [g/mol]:	257.12
CAS:	1564-64-3

Physical Properties

Property code	Value	Unit	Source
ea	0.61 ± 0.10	eV	NIST Webbook
gf	387.77	kJ/mol	Joback Method
hf	289.77	kJ/mol	Joback Method
hfus	24.60	kJ/mol	Joback Method
hvap	60.07	kJ/mol	Joback Method
ie	7.48 ± 0.03	eV	NIST Webbook
ie	7.58	eV	NIST Webbook
log10ws	-6.24		Crippen Method
logp	4.755		Crippen Method
mcvol	162.940	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
rinpol	2143.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2125.00		NIST Webbook
tb	660.48	K	Joback Method
tc	927.78	K	Joback Method
tf	374.15	K	Thermochemical and vapor pressure behavior of anthracene and brominated anthracene mixtures
vc	0.618	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.67	J/molxK	660.48	Joback Method
cpg	380.45	J/molxK	705.03	Joback Method
cpg	392.09	J/molxK	749.58	Joback Method
cpg	402.76	J/molxK	794.13	Joback Method
cpg	412.64	J/molxK	838.68	Joback Method
cpg	421.90	J/molxK	883.23	Joback Method
cpg	430.71	J/molxK	927.78	Joback Method
dvisc	0.0014982	Paxs	424.20	Joback Method
dvisc	0.0011666	Paxs	463.58	Joback Method
dvisc	0.0009447	Paxs	502.96	Joback Method
dvisc	0.0007888	Paxs	542.34	Joback Method
dvisc	0.0006749	Paxs	581.72	Joback Method
dvisc	0.0005890	Paxs	621.10	Joback Method
dvisc	0.0005224	Paxs	660.48	Joback Method
hsubt	100.50 ± 1.80	kJ/mol	341.50	NIST Webbook
psub	1.87e-05	kPa	325.50	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	9.70e-06	kPa	319.00	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub	1.16e-05	kPa	321.80	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.57e-05	kPa	322.90	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	6.00e-06	kPa	315.60	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	2.95e-05	kPa	329.20	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	3.40e-05	kPa	330.80	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub	4.79e-05	kPa	333.10	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	6.28e-05	kPa	336.20	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	9.05e-05	kPa	339.20	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	9.04e-05	kPa	339.90	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	9.19e-05	kPa	340.00	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub	1.02e-04	kPa	342.10	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.16e-04	kPa	342.30	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.36e-04	kPa	344.10	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.41e-04	kPa	344.30	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	2.08e-04	kPa	347.10	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub	2.29e-04	kPa	348.20	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	3.53e-04	kPa	352.10	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	4.50e-04	kPa	355.70	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	8.30e-04	kPa	362.80	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	9.66e-04	kPa	364.00	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub

1.48e-03

kPa

367.80

The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1564643&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemical and vapor pressure behavior of anthracene and brominated anthracene mixtures:	https://www.doi.org/10.1016/j.fluid.2012.12.036
The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique:	https://www.doi.org/10.1016/j.jct.2007.09.006
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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