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	7.58	eV	NIST Webbook
ie	7.48 ± 0.03	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	2125.00		NIST Webbook
rinpol	2143.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2125.00		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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.67	J/mol×K	660.48	Joback Method
cpg	380.45	J/mol×K	705.03	Joback Method
cpg	392.09	J/mol×K	749.58	Joback Method
cpg	402.76	J/mol×K	794.13	Joback Method
cpg	412.64	J/mol×K	838.68	Joback Method
cpg	421.90	J/mol×K	883.23	Joback Method
cpg	430.71	J/mol×K	927.78	Joback Method
dvisc	0.0014982	Pa×s	424.20	Joback Method
dvisc	0.0011666	Pa×s	463.58	Joback Method
dvisc	0.0009447	Pa×s	502.96	Joback Method
dvisc	0.0007888	Pa×s	542.34	Joback Method
dvisc	0.0006749	Pa×s	581.72	Joback Method
dvisc	0.0005890	Pa×s	621.10	Joback Method
dvisc	0.0005224	Pa×s	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

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
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/ci990307l
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

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