

Anthracene, 9,10-dibromo-

Other names:	9,10-dibromoanthracene
Inchi:	InChI=1S/C14H8Br2/c15-13-9-5-1-2-6-10(9)14(16)12-8-4-3-7-11(12)13/h1-8H
InchiKey:	BRUOAURMAFDGLP-UHFFFAOYSA-N
Formula:	C14H8Br2
SMILES:	BrC1c2ccccc2c(Br)c2ccccc12
Mol. weight [g/mol]:	336.02
CAS:	523-27-3

Physical Properties

Property code	Value	Unit	Source
gf	392.46	kJ/mol	Joback Method
hf	304.63	kJ/mol	Joback Method
hfus	29.50	kJ/mol	Joback Method
hvap	67.17	kJ/mol	Joback Method
ie	7.58	eV	NIST Webbook
log10ws	-7.41		Crippen Method
logp	5.518		Crippen Method
mcvol	180.440	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	731.62	K	Joback Method
tc	1010.40	K	Joback Method
tf	496.52	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.48	J/molxK	1010.40	Joback Method
cpg	406.63	J/molxK	778.08	Joback Method
cpg	416.70	J/molxK	824.55	Joback Method
cpg	426.12	J/molxK	871.01	Joback Method
cpg	435.09	J/molxK	917.48	Joback Method
cpg	443.81	J/molxK	963.94	Joback Method
cpg	395.70	J/molxK	731.62	Joback Method

dvisc	0.0013354	Paxs	496.52	Joback Method
dvisc	0.0010734	Paxs	535.70	Joback Method
dvisc	0.0008888	Paxs	574.89	Joback Method
dvisc	0.0007540	Paxs	614.07	Joback Method
dvisc	0.0006523	Paxs	653.25	Joback Method
dvisc	0.0005737	Paxs	692.44	Joback Method
dvisc	0.0005115	Paxs	731.62	Joback Method
hsubt	114.20 ± 2.80	kJ/mol	375.00	NIST Webbook
psub	9.64e-05	kPa	381.90	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	9.23e-05	kPa	381.70	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.42e-04	kPa	386.40	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	391.70	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	381.30	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	6.55e-05	kPa	378.30	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	6.30e-05	kPa	377.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	5.46e-05	kPa	377.20	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	4.45e-05	kPa	373.80	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub	3.94e-05	kPa	372.80	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	2.97e-05	kPa	369.70	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	2.55e-05	kPa	368.70	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.67e-05	kPa	365.50	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.71e-05	kPa	364.90	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub	1.26e-05	kPa	361.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.03e-05	kPa	360.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	9.00e-06	kPa	359.10	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.33e-04	kPa	386.10	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

Sources

- Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
- Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
- 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>

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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