

9,10-Dibromo anthracene

Inchi:	InChI=1S/C14H8Br2/c15-12-7-3-5-10-8-9-4-1-2-6-11(9)14(16)13(10)12/h1-8H
InchiKey:	QBAJKUMKRXROET-UHFFFAOYSA-N
Formula:	C14H8Br2
SMILES:	BrC1cccc2cc3ccccc3c(Br)c12
Mol. weight [g/mol]:	336.02

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
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.70	J/mol×K	731.62	Joback Method
cpg	443.81	J/mol×K	963.94	Joback Method
cpg	435.09	J/mol×K	917.48	Joback Method
cpg	426.12	J/mol×K	871.01	Joback Method
cpg	416.70	J/mol×K	824.55	Joback Method
cpg	406.63	J/mol×K	778.08	Joback Method
cpg	452.48	J/mol×K	1010.40	Joback Method
dvisc	0.0005115	Paxs	731.62	Joback Method
dvisc	0.0005737	Paxs	692.44	Joback Method
dvisc	0.0006523	Paxs	653.25	Joback Method

dvisc	0.0007540	Paxs	614.07	Joback Method
dvisc	0.0008888	Paxs	574.89	Joback Method
dvisc	0.0010734	Paxs	535.70	Joback Method
dvisc	0.0013354	Paxs	496.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000446&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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