

2,6-dibromo-dibenzofuran

Inchi:	InChI=1S/C12H6Br2O2/c13-7-4-5-9-11(6-7)15-10-3-1-2-8(14)12(10)16-9/h1-6H
InchiKey:	JBAGOCOYBUKMHH-UHFFFAOYSA-N
Formula:	C12H6Br2O2
SMILES:	BrC1ccc2c(c1)Oc1cccc(Br)c1O2
Mol. weight [g/mol]:	341.98

Physical Properties

Property code	Value	Unit	Source
gf	173.42	kJ/mol	Joback Method
hf	24.13	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	71.45	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	5.110		Crippen Method
mcvol	168.300	ml/mol	McGowan Method
pc	4385.77	kPa	Joback Method
rinpol	2156.00		NIST Webbook
rinpol	2156.00		NIST Webbook
tb	740.60	K	Joback Method
tc	1020.08	K	Joback Method
tf	526.36	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.39	J/molxK	740.60	Joback Method
cpg	413.49	J/molxK	973.50	Joback Method
cpg	406.06	J/molxK	926.92	Joback Method
cpg	398.41	J/molxK	880.34	Joback Method
cpg	390.37	J/molxK	833.76	Joback Method
cpg	381.75	J/molxK	787.18	Joback Method
cpg	420.88	J/molxK	1020.08	Joback Method
dvisc	0.0005007	Paxs	740.60	Joback Method

dvisc	0.0005680	Paxs	704.89	Joback Method
dvisc	0.0006531	Paxs	669.19	Joback Method
dvisc	0.0007629	Paxs	633.48	Joback Method
dvisc	0.0009077	Paxs	597.77	Joback Method
dvisc	0.0011043	Paxs	562.07	Joback Method
dvisc	0.0013795	Paxs	526.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R171930&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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