

1,3,8-tribromo-dibenzo-dioxin

Inchi:	InChI=1S/C12H5Br3O2/c13-6-1-2-9-10(4-6)17-12-8(15)3-7(14)5-11(12)16-9/h1-5H
InchiKey:	NLKFBKPFQWQPPL-UHFFFAOYSA-N
Formula:	C12H5Br3O2
SMILES:	BrC1ccc2c(c1)Oc1c(Br)cc(Br)cc1O2
Mol. weight [g/mol]:	420.88

Physical Properties

Property code	Value	Unit	Source
gf	178.11	kJ/mol	Joback Method
hf	38.99	kJ/mol	Joback Method
hfus	43.95	kJ/mol	Joback Method
hvap	78.54	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	5.872		Crippen Method
mcvol	185.800	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
rinpol	2428.00		NIST Webbook
rinpol	2428.00		NIST Webbook
tb	811.74	K	Joback Method
tc	1100.91	K	Joback Method
tf	598.68	K	Joback Method
vc	0.685	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.63	J/molxK	811.74	Joback Method
cpg	401.75	J/molxK	859.93	Joback Method
cpg	409.45	J/molxK	908.13	Joback Method
cpg	416.95	J/molxK	956.32	Joback Method
cpg	424.43	J/molxK	1004.52	Joback Method
cpg	432.09	J/molxK	1052.71	Joback Method
cpg	440.15	J/molxK	1100.91	Joback Method
dvisc	0.0010748	Paxs	598.68	Joback Method

dvisc	0.0008850	Paxs	634.19	Joback Method
dvisc	0.0007439	Paxs	669.70	Joback Method
dvisc	0.0006363	Paxs	705.21	Joback Method
dvisc	0.0005525	Paxs	740.72	Joback Method
dvisc	0.0004860	Paxs	776.23	Joback Method
dvisc	0.0004323	Paxs	811.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172493&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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