

Dibenzodioxin, 1,3,7-tribromo-, 9-chloro-

Inchi:	InChI=1S/C12H4Br3ClO2/c13-5-1-7(15)11-9(3-5)17-10-4-6(14)2-8(16)12(10)18-11/h1-4H
InchiKey:	PPVLBMUFMMZHIS-UHFFFAOYSA-N
Formula:	C12H4Br3ClO2
SMILES:	Clc1cc(Br)cc2c1Oc1c(Br)cc(Br)cc1O2
Mol. weight [g/mol]:	455.32

Physical Properties

Property code	Value	Unit	Source
gf	156.55	kJ/mol	Joback Method
hf	11.78	kJ/mol	Joback Method
hfus	47.76	kJ/mol	Joback Method
hvap	83.59	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.526		Crippen Method
mcvol	198.040	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
rinpol	2608.00		NIST Webbook
rinpol	2608.00		NIST Webbook
tb	854.15	K	Joback Method
tc	1144.33	K	Joback Method
tf	641.12	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.09	J/molxK	854.15	Joback Method
cpg	414.50	J/molxK	902.51	Joback Method
cpg	421.68	J/molxK	950.88	Joback Method
cpg	428.84	J/molxK	999.24	Joback Method
cpg	436.15	J/molxK	1047.60	Joback Method
cpg	443.83	J/molxK	1095.96	Joback Method
cpg	452.05	J/molxK	1144.33	Joback Method
dvisc	0.0009125	Paxs	641.12	Joback Method

dvisc	0.0007623	Paxs	676.62	Joback Method
dvisc	0.0006483	Paxs	712.13	Joback Method
dvisc	0.0005599	Paxs	747.63	Joback Method
dvisc	0.0004901	Paxs	783.14	Joback Method
dvisc	0.0004339	Paxs	818.64	Joback Method
dvisc	0.0003881	Paxs	854.15	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R316940&Units=SI

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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