Dibenzodioxin, 2,8-dibromo-, 3,7-dichloro-

Inchi: InChI=1S/C12H3Br2Cl3O2/c13-4-1-7-8(2-5(4)15)18-9-3-6(16)10(14)11(17)12(9)19-7/h1-
InchiKey: GNJKWCIAEOGLTR-UHFFFAOYSA-N
Formula: C12H3Br2Cl3O2
SMILES: Clc1cc2c(cc1Br)Oc1c(cc(Cl)c(Br)c1Cl)O2
Mol. weight [g/mol]: 445.32

Physical Properties

Property code	Value	Unit	Source
gf	108.74	kJ/mol	Joback Method
hf	-57.50	kJ/mol	Joback Method
hfus	50.48	kJ/mol	Joback Method
hvap	86.59	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	7.070		Crippen Method
mcvol	205.020	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
rinpol	2582.00		NIST Webbook
tb	867.83	K	Joback Method
tc	1151.65	K	Joback Method
tf	653.68	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.87	J/mol×K	867.83	Joback Method
cpg	421.66	J/mol×K	915.13	Joback Method
cpg	428.23	J/mol×K	962.44	Joback Method
cpg	434.72	J/mol×K	1009.74	Joback Method
cpg	441.28	J/mol×K	1057.04	Joback Method
cpg	448.08	J/mol×K	1104.35	Joback Method
cpg	455.26	J/mol×K	1151.65	Joback Method
dvisc	0.0008645	Pa×s	653.68	Joback Method
dvisc	0.0007260	Pa×s	689.37	Joback Method

dvisc	0.0006203	Pa×s	725.06	Joback Method
dvisc	0.0005379	Pa×s	760.76	Joback Method
dvisc	0.0004724	Pa×s	796.45	Joback Method
dvisc	0.0004195	Pa×s	832.14	Joback Method
dvisc	0.0003762	Pa×s	867.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R317374&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
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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