dibenzodioxin, 1-bromo-, 2,3,4,7,8-pentachloro-

Inchi: InChI=1S/C12H2BrCl5O2/c13-7-8(16)9(17)10(18)12-11(7)19-5-1-3(14)4(15)2-6(5)20-12/

InchiKey: QVVLEISUOPFQTL-UHFFFAOYSA-N

Formula: C12H2BrCl5O2

SMILES: Clc1cc2c(cc1Cl)Oc1c(Br)c(Cl)c(Cl)c(Cl)c1O2

Mol. weight [g/mol]: 435.31

Physical Properties

Property code	Value	Unit	Source
gf	60.93	kJ/mol	Joback Method
hf	-126.78	kJ/mol	Joback Method
hfus	53.20	kJ/mol	Joback Method
hvap	89.58	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	7.614		Crippen Method
mcvol	212.000	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	2852.00		NIST Webbook
tb	881.51	K	Joback Method
tc	1159.42	K	Joback Method
tf	666.24	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.41	J/mol×K	881.51	Joback Method
cpg	428.61	J/mol×K	927.83	Joback Method
cpg	434.56	J/mol×K	974.15	Joback Method
cpg	440.37	J/mol×K	1020.46	Joback Method
cpg	446.17	J/mol×K	1066.78	Joback Method
cpg	452.08	J/mol×K	1113.10	Joback Method
cpg	458.23	J/mol×K	1159.42	Joback Method
dvisc	0.0008204	Pa×s	666.24	Joback Method
dvisc	0.0006924	Pa×s	702.12	Joback Method

dvisc	0.0005942	Pa×s	738.00	Joback Method
dvisc	0.0005171	Pa×s	773.88	Joback Method
dvisc	0.0004556	Pa×s	809.75	Joback Method
dvisc	0.0004058	Pa×s	845.63	Joback Method
dvisc	0.0003648	Pa×s	881.51	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R317161&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