Dibenzodioxin, 1-bromo-, 3,8-dichloro-

Other names: 1-bromo-3,8-dichloro-dibenzo-p-dioxin
Inchi: InChI=1S/C12H5BrCl2O2/c13-8-3-7(15)5-11-12(8)17-10-4-6(14)1-2-9(10)16-11/h1-5H
InchiKey: KXISDFSRMWASLH-UHFFFAOYSA-N
Formula: C12H5BrCl2O2
SMILES: Clc1ccc2c(c1)Oc1c(Br)cc(Cl)cc1O2
Mol. weight [g/mol]: 331.98

Physical Properties

Property code	Value	Unit	Source
gf	125.61	kJ/mol	Joback Method
hf	-45.15	kJ/mol	Joback Method
hfus	41.77	kJ/mol	Joback Method
hvap	74.44	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.654		Crippen Method
mcvol	175.280	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
tb	754.28	K	Joback Method
tc	1027.42	K	Joback Method
tf	538.92	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.64	J/mol×K	754.28	Joback Method
cpg	390.26	J/mol×K	799.80	Joback Method
cpg	398.22	J/mol×K	845.33	Joback Method
cpg	405.64	J/mol×K	890.85	Joback Method
cpg	412.67	J/mol×K	936.37	Joback Method
cpg	419.46	J/mol×K	981.90	Joback Method

cpg	426.14	J/mol×K	1027.42	Joback Method
dvisc	0.0012797	Pa×s	538.92	Joback Method
dvisc	0.0010327	Pa×s	574.81	Joback Method
dvisc	0.0008547	Pa×s	610.71	Joback Method
dvisc	0.0007224	Pa×s	646.60	Joback Method
dvisc	0.0006214	Pa×s	682.49	Joback Method
dvisc	0.0005427	Pa×s	718.39	Joback Method
dvisc	0.0004801	Pa×s	754.28	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R171569&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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