Dibenzodioxin, 4-bromo-, 1,2,7,8-tetrachloro-

Other names: 4-bromo-1,2,7,8-tetrachloro-dibenzo-p-dioxin
Dibenzodioxin, 4-bromo-, 1,2,8,9-tetrachloro-
Inchi: InChI=1S/C12H3BrCl4O2/c13-4-1-7(16)10(17)12-11(4)18-8-2-5(14)6(15)3-9(8)19-12/h1-
InchiKey: LIJLFIDUAFUCRA-UHFFFAOYSA-N
Formula: C12H3BrCl4O2
SMILES: Clc1cc2c(cc1Cl)Oc1c(Cl)c(Cl)cc(Br)c1O2
Mol. weight [g/mol]: 400.87

Physical Properties

Property code	Value	Unit	Source
gf	82.49	kJ/mol	Joback Method
hf	-99.57	kJ/mol	Joback Method
hfus	49.39	kJ/mol	Joback Method
hvap	84.54	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.961		Crippen Method
mcvol	199.760	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	2612.00		NIST Webbook
rinpol	2612.00		NIST Webbook
rinpol	2612.00		NIST Webbook
rinpol	2627.00		NIST Webbook
tb	839.10	K	Joback Method
tc	1115.62	K	Joback Method
tf	623.80	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.99	J/mol×K	839.10	Joback Method
cpg	441.80	J/mol×K	1069.53	Joback Method
cpg	435.68	J/mol×K	1023.45	Joback Method
cpg	429.57	J/mol×K	977.36	Joback Method

cpg	423.34	J/mol×K	931.27	Joback Method
cpg	416.86	J/mol×K	885.19	Joback Method
cpg	448.04	J/mol×K	1115.62	Joback Method
dvisc	0.0004037	Pa×s	839.10	Joback Method
dvisc	0.0004512	Pa×s	803.22	Joback Method
dvisc	0.0005097	Pa×s	767.33	Joback Method
dvisc	0.0005825	Pa×s	731.45	Joback Method
dvisc	0.0006751	Pa×s	695.57	Joback Method
dvisc	0.0007950	Pa×s	659.68	Joback Method
dvisc	0.0009540	Pa×s	623.80	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R172220&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

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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