

3-bromo-1,2,6,9-tetrachloro-dibenzo-p-dioxin

Other names:	Dibenzodioxin, 3-bromo-, 1,2,6,9-tetrachloro-
Inchi:	InChI=1S/C12H3BrCl4O2/c13-4-3-7-12(9(17)8(4)16)19-11-6(15)2-1-5(14)10(11)18-7/h1-
InchiKey:	UNOFFEISMYTOSE-UHFFFAOYSA-N
Formula:	C12H3BrCl4O2
SMILES:	Clc1ccc(Cl)c2c1Oc1cc(Br)c(Cl)c(Cl)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	2638.00		NIST Webbook
rinpol	2638.00		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/molxK	839.10	Joback Method
cpg	416.86	J/molxK	885.19	Joback Method
cpg	423.34	J/molxK	931.27	Joback Method
cpg	429.57	J/molxK	977.36	Joback Method
cpg	435.68	J/molxK	1023.45	Joback Method
cpg	441.80	J/molxK	1069.53	Joback Method
cpg	448.04	J/molxK	1115.62	Joback Method

dvisc	0.0009540	Paxs	623.80	Joback Method
dvisc	0.0007950	Paxs	659.68	Joback Method
dvisc	0.0006751	Paxs	695.57	Joback Method
dvisc	0.0005825	Paxs	731.45	Joback Method
dvisc	0.0005097	Paxs	767.33	Joback Method
dvisc	0.0004512	Paxs	803.22	Joback Method
dvisc	0.0004037	Paxs	839.10	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=R172151&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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