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/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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172151&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

Latest version available from:
https://www.chemeo.com/cid/48-639-0/3-bromo-1-2-6-9-tetrachloro-dibenzo-p-dioxin.pdf
Generated by Cheméo on 2024-10-12 08:56:00.514289983 +0000 UTC m=+3304223.151259232.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.