2,3,7,8-tetrabromodibenzo-dioxin

Other names: 2,3,7,8-Tetrabromodibenzo-p-dioxin
Inchi: InChI=1S/C12H4Br4O2/c13-5-1-9-10(2-6(5)14)18-12-4-8(16)7(15)3-11(12)17-9/h1-4H
InchiKey: JZLQUWSWOJPCAK-UHFFFAOYSA-N
Formula: C12H4Br4O2
SMILES: Brc1cc2c(cc1Br)Oc1cc(Br)c(Br)cc1O2
Mol. weight [g/mol]: 499.77

Physical Properties

Property code	Value	Unit	Source
gf	182.80	kJ/mol	Joback Method
hf	53.85	kJ/mol	Joback Method
hfus	48.85	kJ/mol	Joback Method
hvap	85.64	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.635		Crippen Method
mcvol	203.300	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
rinpol	2821.00		NIST Webbook
rinpol	2821.00		NIST Webbook
rinpol	2822.00		NIST Webbook
rinpol	2821.00		NIST Webbook
tb	882.88	K	Joback Method
tc	1180.48	K	Joback Method
tf	671.00	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.07	J/mol×K	882.88	Joback Method
cpg	419.55	J/mol×K	932.48	Joback Method
cpg	427.01	J/mol×K	982.08	Joback Method
cpg	434.69	J/mol×K	1031.68	Joback Method
cpg	442.80	J/mol×K	1081.28	Joback Method

cpg	451.58	J/mol×K	1130.88	Joback Method
cpg	461.26	J/mol×K	1180.48	Joback Method
dvisc	0.0008138	Pa×s	671.00	Joback Method
dvisc	0.0006851	Pa×s	706.31	Joback Method
dvisc	0.0005863	Pa×s	741.63	Joback Method
dvisc	0.0005088	Pa×s	776.94	Joback Method
dvisc	0.0004471	Pa×s	812.25	Joback Method
dvisc	0.0003971	Pa×s	847.57	Joback Method
dvisc	0.0003561	Pa×s	882.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R171747&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