1,2,3,4-Tetrabromodibenzo-p-dioxin

Other names: 1,2,3,4-tetrabromodibenzodioxin
Inchi: InChI=1S/C12H4Br4O2/c13-7-8(14)10(16)12-11(9(7)15)17-5-3-1-2-4-6(5)18-12/h1-4H
InchiKey: AKUPIABWVUYZPX-UHFFFAOYSA-N
Formula: C12H4Br4O2
SMILES: Brc1c(Br)c(Br)c2c(c1Br)Oc1ccccc1O2
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	2811.00		NIST Webbook
rinpol	2765.00		NIST Webbook
rinpol	2811.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R170526&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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