1,3,7-tribromo-dibenzo-dioxin

Inchi: InChI=1S/C12H5Br3O2/c13-6-1-2-9-10(4-6)16-11-5-7(14)3-8(15)12(11)17-9/h1-5H
InchiKey: RIATZSLLGBMQMM-UHFFFAOYSA-N
Formula: C12H5Br3O2
SMILES: Brc1ccc2c(c1)Oc1cc(Br)cc(Br)c1O2
Mol. weight [g/mol]: 420.88

Physical Properties

Property code	Value	Unit	Source
gf	178.11	kJ/mol	Joback Method
hf	38.99	kJ/mol	Joback Method
hfus	43.95	kJ/mol	Joback Method
hvap	78.54	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	5.872		Crippen Method
mcvol	185.800	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
rinpol	2428.00		NIST Webbook
rinpol	2428.00		NIST Webbook
tb	811.74	K	Joback Method
tc	1100.91	K	Joback Method
tf	598.68	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.63	J/mol×K	811.74	Joback Method
cpg	401.75	J/mol×K	859.93	Joback Method
cpg	409.45	J/mol×K	908.13	Joback Method
cpg	416.95	J/mol×K	956.32	Joback Method
cpg	424.43	J/mol×K	1004.52	Joback Method
cpg	432.09	J/mol×K	1052.71	Joback Method
cpg	440.15	J/mol×K	1100.91	Joback Method
dvisc	0.0010748	Pa×s	598.68	Joback Method

dvisc	0.0008850	Pa×s	634.19	Joback Method
dvisc	0.0007439	Pa×s	669.70	Joback Method
dvisc	0.0006363	Pa×s	705.21	Joback Method
dvisc	0.0005525	Pa×s	740.72	Joback Method
dvisc	0.0004860	Pa×s	776.23	Joback Method
dvisc	0.0004323	Pa×s	811.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172488&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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