1,2,4,6,8-pentabromo-dibenzo-dioxin

Inchi: InChI=1S/C12H3Br5O2/c13-4-1-6(15)10-8(2-4)18-12-9(17)5(14)3-7(16)11(12)19-10/h1-3
InchiKey: FPGDCFSGMHTTLK-UHFFFAOYSA-N
Formula: C12H3Br5O2
SMILES: Brc1cc(Br)c2c(c1)Oc1c(Br)c(Br)cc(Br)c1O2
Mol. weight [g/mol]: 578.67

Physical Properties

Property code	Value	Unit	Source
gf	187.49	kJ/mol	Joback Method
hf	68.71	kJ/mol	Joback Method
hfus	53.74	kJ/mol	Joback Method
hvap	92.74	kJ/mol	Joback Method
log10ws	-8.80		Crippen Method
logp	7.397		Crippen Method
mcvol	220.800	ml/mol	McGowan Method
pc	5503.26	kPa	Joback Method
rinpol	3071.00		NIST Webbook
rinpol	3071.00		NIST Webbook
tb	954.02	K	Joback Method
tc	1259.09	K	Joback Method
tf	743.32	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.97	J/mol×K	954.02	Joback Method
cpg	436.52	J/mol×K	1004.86	Joback Method
cpg	444.52	J/mol×K	1055.71	Joback Method
cpg	453.23	J/mol×K	1106.55	Joback Method
cpg	462.89	J/mol×K	1157.40	Joback Method
cpg	473.76	J/mol×K	1208.24	Joback Method
cpg	486.09	J/mol×K	1259.09	Joback Method
dvisc	0.0006039	Pa×s	743.32	Joback Method

dvisc	0.0005175	Pa×s	778.44	Joback Method
dvisc	0.0004494	Pa×s	813.55	Joback Method
dvisc	0.0003948	Pa×s	848.67	Joback Method
dvisc	0.0003505	Pa×s	883.79	Joback Method
dvisc	0.0003140	Pa×s	918.90	Joback Method
dvisc	0.0002835	Pa×s	954.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172359&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