Octane, 2,3-bis-(trichloromethyl)

Inchi: InChI=1S/C10H16Cl6/c1-3-4-5-6-8(10(14,15)16)7(2)9(11,12)13/h7-8H,3-6H2,1-2H3
InchiKey: JYFLTEYKFGSUIS-UHFFFAOYSA-N
Formula: C10H16Cl6
SMILES: CCCCCC(C(C)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 348.95

Physical Properties

Property code	Value	Unit	Source
gf	-37.46	kJ/mol	Joback Method
hf	-372.23	kJ/mol	Joback Method
hfus	24.96	kJ/mol	Joback Method
hvap	60.80	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	6.559		Crippen Method
mcvol	225.200	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	1774.00		NIST Webbook
rinpol	1774.00		NIST Webbook
tb	645.44	K	Joback Method
tc	867.32	K	Joback Method
tf	356.82	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.22	J/mol×K	645.44	Joback Method
cpg	511.90	J/mol×K	682.42	Joback Method
cpg	523.57	J/mol×K	719.40	Joback Method
cpg	534.32	J/mol×K	756.38	Joback Method
cpg	544.25	J/mol×K	793.36	Joback Method
cpg	553.45	J/mol×K	830.34	Joback Method
cpg	562.01	J/mol×K	867.32	Joback Method
dvisc	0.0039773	Pa×s	356.82	Joback Method

dvisc	0.0015468	Pa×s	404.92	Joback Method
dvisc	0.0007351	Pa×s	453.03	Joback Method
dvisc	0.0004030	Pa×s	501.13	Joback Method
dvisc	0.0002455	Pa×s	549.23	Joback Method
dvisc	0.0001620	Pa×s	597.34	Joback Method
dvisc	0.0001137	Pa×s	645.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515469&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