1,1,1,2,3,3,3-HEPTACHLOROPROPANE

Inchi: InChI=1S/C3HCl7/c4-1(2(5,6)7)3(8,9)10/h1H
InchiKey: LZOUTMTXULWVSU-UHFFFAOYSA-N
Formula: C3HCl7
SMILES: ClC(C(Cl)(Cl)Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 285.21

Physical Properties

Property code	Value	Unit	Source
gf	-105.89	kJ/mol	Joback Method
hf	-210.02	kJ/mol	Cheméo Relay (1.0)
hfus	14.55	kJ/mol	Joback Method
hvap	59.05	kJ/mol	Cheméo Relay (1.0)
ie	10.86	eV	Cheméo Relay (1.0)
log10ws	-3.77		Cheméo Relay (1.0)
logp	4.334		Crippen Method
mcvol	138.810	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
rinpol	1380.00		NIST Webbook
rinpol	1380.00		NIST Webbook
tb	505.42	K	Cheméo Relay (1.0)
tc	716.93	K	Cheméo Relay (1.0)
tf	274.69	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.37	J/mol×K	523.15	Joback Method
cpg	216.21	J/mol×K	565.51	Joback Method
cpg	220.21	J/mol×K	607.87	Joback Method
cpg	223.45	J/mol×K	650.24	Joback Method
cpg	226.06	J/mol×K	692.60	Joback Method
cpg	228.13	J/mol×K	734.96	Joback Method
cpg	229.76	J/mol×K	777.32	Joback Method
dvisc	0.0050546	Pa×s	322.85	Joback Method

dvisc	0.0025844	Pa×s	356.23	Joback Method
dvisc	0.0014823	Pa×s	389.62	Joback Method
dvisc	0.0009282	Pa×s	423.00	Joback Method
dvisc	0.0006224	Pa×s	456.38	Joback Method
dvisc	0.0004407	Pa×s	489.77	Joback Method
dvisc	0.0003261	Pa×s	523.15	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3849330&Units=SI
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
ie:	Ionization energy
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

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