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

Other names:	ASYM-HEPTACHLOROPROPANE
	Propane, 1,1,1,2,2,3,3-heptachloro-
Inchi:	InChI=1S/C3HCl7/c4-1(5)2(6,7)3(8,9)10/h1H
InchiKey:	YFIIENAGGCUHIQ-UHFFFAOYSA-N
Formula:	C3HCl7
SMILES:	ClC(Cl)C(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	-176.19	kJ/mol	Cheméo Relay (1.0)
hfus	14.55	kJ/mol	Joback Method
hvap	61.96	kJ/mol	Cheméo Relay (1.0)
ie	11.04	eV	Cheméo Relay (1.0)
log10ws	-3.92		Cheméo Relay (1.0)
logp	4.334		Crippen Method
mcvol	138.810	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
tb	520.70	K	NIST Webbook
tc	752.40	K	Cheméo Relay (1.0)
tf	330.82	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.13	J/mol×K	734.96	Joback Method
cpg	229.76	J/mol×K	777.32	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	211.37	J/mol×K	523.15	Joback Method
dvisc	0.0014823	Pa×s	389.62	Joback Method

dvisc	0.0025844	Pa×s	356.23	Joback Method
dvisc	0.0050546	Pa×s	322.85	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
hvapt	34.80	kJ/mol	443.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	438.70	K	12.00	NIST Webbook
tbrp	405.20	K	4.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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):
KDB: https://www.cheric.org/files/research/kdb/mol/mol1582.mol
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C594898&Units=SI
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
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point