OCTACHLOROPROPANE

Other names: Propane, octachloro-
Inchi: InChI=1S/C3Cl8/c4-1(5,2(6,7)8)3(9,10)11
InchiKey: QQAHAGNPDBPSJP-UHFFFAOYSA-N
Formula: C3Cl8
SMILES: ClC(Cl)(Cl)C(Cl)(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 319.66

Physical Properties

Property code	Value	Unit	Source
af	0.2789		Cheméo Relay (1.0)
hf	-179.20	kJ/mol	Cheméo Relay (1.0)
hfus	14.86	kJ/mol	Joback Method
hvap	61.50	kJ/mol	Cheméo Relay (1.0)
ie	10.93	eV	Cheméo Relay (1.0)
log10ws	-4.63		Cheméo Relay (1.0)
logp	4.901		Crippen Method
mcvol	151.050	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
rinpol	1580.00		NIST Webbook
tb	525.40	K	Cheméo Relay (1.0)
tc	757.31	K	Cheméo Relay (1.0)
tf	408.32	K	Cheméo Relay (1.0)
vc	0.520	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.49	J/mol×K	557.79	Joback Method
cpg	235.40	J/mol×K	602.83	Joback Method
cpg	238.28	J/mol×K	647.88	Joback Method
cpg	240.30	J/mol×K	692.92	Joback Method
cpg	241.64	J/mol×K	737.96	Joback Method
cpg	242.46	J/mol×K	783.01	Joback Method
cpg	242.94	J/mol×K	828.05	Joback Method

dvisc	0.0031121	Pa×s	370.19	Joback Method
dvisc	0.0017690	Pa×s	401.46	Joback Method
dvisc	0.0010910	Pa×s	432.72	Joback Method
dvisc	0.0007182	Pa×s	463.99	Joback Method
dvisc	0.0004984	Pa×s	495.26	Joback Method
dvisc	0.0003612	Pa×s	526.52	Joback Method
dvisc	0.0002714	Pa×s	557.79	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C594901&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
vc: Critical Volume

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