threo-2,3-dichloropentane

Other names: 2,3-dichloropentane (threo)
Pentane, 2,3-dichloro-, threo
Inchi: InChI=1S/C5H10Cl2/c1-3-5(7)4(2)6/h4-5H,3H2,1-2H3/t4-,5+/m0/s1
InchiKey: HVFJQRZGBBKTPL-CRCLSJGQSA-N
Formula: C5H10Cl2
SMILES: CCC(Cl)C(C)Cl
Mol. weight [g/mol]: 141.04

Physical Properties

Property code	Value	Unit	Source
gf	-37.52	kJ/mol	Joback Method
hf	-188.57	kJ/mol	Joback Method
hfus	10.05	kJ/mol	Joback Method
hvap	34.72	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.631		Crippen Method
mcvol	105.790	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	895.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	895.00		NIST Webbook
ripol	1192.00		NIST Webbook
tb	387.78	K	Joback Method
tc	577.75	K	Joback Method
tf	175.95	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.68	J/mol×K	387.78	Joback Method
cpg	218.66	J/mol×K	546.09	Joback Method
cpg	210.87	J/mol×K	514.43	Joback Method
cpg	202.69	J/mol×K	482.77	Joback Method

cpg	194.11	J/mol×K	451.10	Joback Method
cpg	185.11	J/mol×K	419.44	Joback Method
cpg	226.08	J/mol×K	577.75	Joback Method
dvisc	0.0003189	Pa×s	387.78	Joback Method
dvisc	0.0004347	Pa×s	352.48	Joback Method
dvisc	0.0006349	Pa×s	317.17	Joback Method
dvisc	0.0010197	Pa×s	281.87	Joback Method
dvisc	0.0018754	Pa×s	246.56	Joback Method
dvisc	0.0042286	Pa×s	211.25	Joback Method
dvisc	0.0132129	Pa×s	175.95	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R211875&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume