4-Heptanone, 3,5-dichloro (RS, SR)

Inchi: InChI=1S/C7H12Cl2O/c1-3-5(8)7(10)6(9)4-2/h5-6H,3-4H2,1-2H3
InchiKey: PAHVFZSVIQBSNV-UHFFFAOYSA-N
Formula: C7H12Cl2O
SMILES: CCC(Cl)C(=O)C(Cl)CC
Mol. weight [g/mol]: 183.08

Physical Properties

Property code	Value	Unit	Source
gf	-149.60	kJ/mol	Joback Method
hf	-342.43	kJ/mol	Joback Method
hfus	16.83	kJ/mol	Joback Method
hvap	45.92	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.590		Crippen Method
mcvol	135.540	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	1072.00		NIST Webbook
rinpol	1072.00		NIST Webbook
tb	487.41	K	Joback Method
tc	685.16	K	Joback Method
tf	248.42	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.72	J/mol×K	487.41	Joback Method
cpg	279.89	J/mol×K	520.37	Joback Method
cpg	290.49	J/mol×K	553.33	Joback Method
cpg	300.54	J/mol×K	586.29	Joback Method
cpg	310.05	J/mol×K	619.25	Joback Method
cpg	319.06	J/mol×K	652.21	Joback Method
cpg	327.56	J/mol×K	685.16	Joback Method
dvisc	0.0077940	Pa×s	248.42	Joback Method

dvisc	0.0031406	Pa×s	288.25	Joback Method
dvisc	0.0015781	Pa×s	328.08	Joback Method
dvisc	0.0009203	Pa×s	367.91	Joback Method
dvisc	0.0005964	Pa×s	407.75	Joback Method
dvisc	0.0004175	Pa×s	447.58	Joback Method
dvisc	0.0003098	Pa×s	487.41	Joback Method

Sources

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=R630563&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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