3-Heptanone, 2,4-dichloro (RR, SS)

Inchi: InChI=1S/C7H12Cl2O/c1-3-4-6(9)7(10)5(2)8/h5-6H,3-4H2,1-2H3
InchiKey: DQJUTHPOQJSEPV-UHFFFAOYSA-N
Formula: C7H12Cl2O
SMILES: CCCC(Cl)C(=O)C(C)Cl
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	1102.00		NIST Webbook
rinpol	1102.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630078&Units=SI
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

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