3-Hexanone, 2,4-dichloro, (RS, SR)

Inchi: InChI=1S/C6H10Cl2O/c1-3-5(8)6(9)4(2)7/h4-5H,3H2,1-2H3
InchiKey: CDOGVHILADCNET-UHFFFAOYSA-N
Formula: C6H10Cl2O
SMILES: CCC(Cl)C(=O)C(C)Cl
Mol. weight [g/mol]: 169.05

Physical Properties

Property code	Value	Unit	Source
gf	-158.02	kJ/mol	Joback Method
hf	-321.79	kJ/mol	Joback Method
hfus	14.24	kJ/mol	Joback Method
hvap	43.69	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.200		Crippen Method
mcvol	121.450	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
rinpol	976.00		NIST Webbook
rinpol	976.00		NIST Webbook
tb	464.53	K	Joback Method
tc	664.81	K	Joback Method
tf	237.15	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.95	J/mol×K	464.53	Joback Method
cpg	237.97	J/mol×K	497.91	Joback Method
cpg	247.47	J/mol×K	531.29	Joback Method
cpg	256.47	J/mol×K	564.67	Joback Method
cpg	265.00	J/mol×K	598.05	Joback Method
cpg	273.06	J/mol×K	631.43	Joback Method
cpg	280.67	J/mol×K	664.81	Joback Method
dvisc	0.0080703	Pa×s	237.15	Joback Method

dvisc	0.0032987	Pa×s	275.05	Joback Method
dvisc	0.0016746	Pa×s	312.94	Joback Method
dvisc	0.0009842	Pa×s	350.84	Joback Method
dvisc	0.0006416	Pa×s	388.74	Joback Method
dvisc	0.0004513	Pa×s	426.63	Joback Method
dvisc	0.0003362	Pa×s	464.53	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=R630201&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume