4-Heptanone, 3,5-dichloro-2,6-dimethyl (RS, SR)

Inchi: InChI=1S/C9H16Cl2O/c1-5(2)7(10)9(12)8(11)6(3)4/h5-8H,1-4H3
InchiKey: ZKGKZMHBQUCLPJ-UHFFFAOYSA-N
Formula: C9H16Cl2O
SMILES: CC(C)C(Cl)C(=O)C(Cl)C(C)C
Mol. weight [g/mol]: 211.13

Physical Properties

Property code	Value	Unit	Source
gf	-137.64	kJ/mol	Joback Method
hf	-394.27	kJ/mol	Joback Method
hfus	14.97	kJ/mol	Joback Method
hvap	49.59	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	3.082		Crippen Method
mcvol	163.720	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1204.00		NIST Webbook
rinpol	1204.00		NIST Webbook
tb	532.29	K	Joback Method
tc	733.28	K	Joback Method
tf	240.96	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.84	J/mol×K	532.29	Joback Method
cpg	370.62	J/mol×K	565.79	Joback Method
cpg	383.66	J/mol×K	599.29	Joback Method
cpg	396.00	J/mol×K	632.78	Joback Method
cpg	407.65	J/mol×K	666.28	Joback Method
cpg	418.64	J/mol×K	699.78	Joback Method
cpg	429.00	J/mol×K	733.28	Joback Method
dvisc	0.0169289	Pa×s	240.96	Joback Method

dvisc	0.0045177	Pa×s	289.51	Joback Method
dvisc	0.0017620	Pa×s	338.07	Joback Method
dvisc	0.0008705	Pa×s	386.62	Joback Method
dvisc	0.0005034	Pa×s	435.18	Joback Method
dvisc	0.0003249	Pa×s	483.73	Joback Method
dvisc	0.0002272	Pa×s	532.29	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=R630543&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