

4-Heptanone, 3,5-dichloro-2,6-dimethyl (RR, SS)

Inchi:	InChI=1S/C9H16Cl2O/c1-5(2)7(10)9(12)8(11)6(3)4/h5-8H,1-4H3
InchiKey:	ZKGGKZMHBQUCLPJ-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
mvol	163.720	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1240.00		NIST Webbook
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tb	532.29	K	Joback Method
tc	733.28	K	Joback Method
tf	240.96	K	Joback Method
vc	0.620	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.84	J/molxK	532.29	Joback Method
cpg	418.64	J/molxK	699.78	Joback Method
cpg	407.65	J/molxK	666.28	Joback Method
cpg	396.00	J/molxK	632.78	Joback Method
cpg	383.66	J/molxK	599.29	Joback Method
cpg	370.62	J/molxK	565.79	Joback Method
cpg	429.00	J/molxK	733.28	Joback Method
dvisc	0.0002272	Paxs	532.29	Joback Method

dvisc	0.0003249	Paxs	483.73	Joback Method
dvisc	0.0005034	Paxs	435.18	Joback Method
dvisc	0.0008705	Paxs	386.62	Joback Method
dvisc	0.0017620	Paxs	338.07	Joback Method
dvisc	0.0045177	Paxs	289.51	Joback Method
dvisc	0.0169289	Paxs	240.96	Joback Method

Sources

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=R630538&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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