

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

Inchi:	InChI=1S/C8H14Cl2O/c1-4-5(2)7(10)8(11)6(3)9/h5-7H,4H2,1-3H3
InchiKey:	KDLBNTUOPSRHRY-UHFFFAOYSA-N
Formula:	C8H14Cl2O
SMILES:	CCC(C)C(Cl)C(=O)C(C)Cl
Mol. weight [g/mol]:	197.10

Physical Properties

Property code	Value	Unit	Source
gf	-143.62	kJ/mol	Joback Method
hf	-368.35	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	47.75	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.836		Crippen Method
mcvol	149.630	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1180.00		NIST Webbook
rinpol	1180.00		NIST Webbook
tb	509.85	K	Joback Method
tc	709.33	K	Joback Method
tf	244.69	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.79	J/molxK	509.85	Joback Method
cpg	324.31	J/molxK	543.10	Joback Method
cpg	336.18	J/molxK	576.34	Joback Method
cpg	347.43	J/molxK	609.59	Joback Method
cpg	358.06	J/molxK	642.84	Joback Method
cpg	368.10	J/molxK	676.09	Joback Method
cpg	377.58	J/molxK	709.33	Joback Method
dvisc	0.0114024	Paxs	244.69	Joback Method

dvisc	0.0037800	Paxs	288.88	Joback Method
dvisc	0.0016797	Paxs	333.08	Joback Method
dvisc	0.0009026	Paxs	377.27	Joback Method
dvisc	0.0005525	Paxs	421.46	Joback Method
dvisc	0.0003712	Paxs	465.66	Joback Method
dvisc	0.0002672	Paxs	509.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630058&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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