

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

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	1011.00		NIST Webbook
rinpol	1011.00		NIST Webbook
tb	464.53	K	Joback Method
tc	664.81	K	Joback Method
tf	237.15	K	Joback Method
vc	0.464	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.95	J/molxK	464.53	Joback Method
cpg	273.06	J/molxK	631.43	Joback Method
cpg	265.00	J/molxK	598.05	Joback Method
cpg	256.47	J/molxK	564.67	Joback Method
cpg	247.47	J/molxK	531.29	Joback Method
cpg	237.97	J/molxK	497.91	Joback Method
cpg	280.67	J/molxK	664.81	Joback Method
dvisc	0.0003362	Paxs	464.53	Joback Method

dvisc	0.0004513	Paxs	426.63	Joback Method
dvisc	0.0006416	Paxs	388.74	Joback Method
dvisc	0.0009842	Paxs	350.84	Joback Method
dvisc	0.0016746	Paxs	312.94	Joback Method
dvisc	0.0032987	Paxs	275.05	Joback Method
dvisc	0.0080703	Paxs	237.15	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630192&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

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