

3-Hexanone, 4,4-dichloro

Inchi:	InChI=1S/C6H10Cl2O/c1-3-5(9)6(7,8)4-2/h3-4H2,1-2H3
InchiKey:	ZQBGKIGYOVBXJP-UHFFFAOYSA-N
Formula:	C6H10Cl2O
SMILES:	CCC(=O)C(Cl)(Cl)CC
Mol. weight [g/mol]:	169.05

Physical Properties

Property code	Value	Unit	Source
gf	-150.30	kJ/mol	Joback Method
hf	-319.98	kJ/mol	Joback Method
hfus	13.88	kJ/mol	Joback Method
hvap	43.17	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.549		Crippen Method
mcvol	121.450	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	935.00		NIST Webbook
rinpol	935.00		NIST Webbook
tb	462.18	K	Joback Method
tc	666.21	K	Joback Method
tf	269.57	K	Joback Method
vc	0.465	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.68	J/mol×K	462.18	Joback Method
cpg	276.51	J/mol×K	632.20	Joback Method
cpg	268.54	J/mol×K	598.20	Joback Method
cpg	260.00	J/mol×K	564.19	Joback Method
cpg	250.87	J/mol×K	530.19	Joback Method
cpg	241.10	J/mol×K	496.18	Joback Method
cpg	283.96	J/mol×K	666.21	Joback Method
dvisc	0.0003744	Paxs	462.18	Joback Method

dvisc	0.0004930	Paxs	430.08	Joback Method
dvisc	0.0006788	Paxs	397.98	Joback Method
dvisc	0.0009885	Paxs	365.88	Joback Method
dvisc	0.0015473	Paxs	333.77	Joback Method
dvisc	0.0026645	Paxs	301.67	Joback Method
dvisc	0.0052226	Paxs	269.57	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=R630221&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

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