

3-Pentanone, 4,4-dichloro-2-methyl

Inchi:	InChI=1S/C6H10Cl2O/c1-4(2)5(9)6(3,7)8/h4H,1-3H3
InchiKey:	TYPXQMUXDUBPF-UHFFFAOYSA-N
Formula:	C6H10Cl2O
SMILES:	CC(C)C(=O)C(C)(Cl)Cl
Mol. weight [g/mol]:	169.05

Physical Properties

Property code	Value	Unit	Source
gf	-152.74	kJ/mol	Joback Method
hf	-325.26	kJ/mol	Joback Method
hfus	10.35	kJ/mol	Joback Method
hvap	42.78	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.405		Crippen Method
mvol	121.450	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
rinpol	886.00		NIST Webbook
rinpol	886.00		NIST Webbook
tb	461.74	K	Joback Method
tc	670.58	K	Joback Method
tf	254.57	K	Joback Method
vc	0.459	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.86	J/molxK	461.74	Joback Method
cpg	241.62	J/molxK	496.55	Joback Method
cpg	251.67	J/molxK	531.35	Joback Method
cpg	261.06	J/molxK	566.16	Joback Method
cpg	269.82	J/molxK	600.97	Joback Method
cpg	277.98	J/molxK	635.77	Joback Method
cpg	285.58	J/molxK	670.58	Joback Method
dvisc	0.0076920	Paxs	254.57	Joback Method

dvisc	0.0033961	Paxs	289.10	Joback Method
dvisc	0.0017852	Paxs	323.63	Joback Method
dvisc	0.0010623	Paxs	358.15	Joback Method
dvisc	0.0006925	Paxs	392.68	Joback Method
dvisc	0.0004838	Paxs	427.21	Joback Method
dvisc	0.0003566	Paxs	461.74	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=R630390&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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