

2-Butanone, 1,3-dichloro-3-methyl

Inchi:	InChI=1S/C5H8Cl2O/c1-5(2,7)4(8)3-6/h3H2,1-2H3
InchiKey:	NEVIWYGONGMZRK-UHFFFAOYSA-N
Formula:	C5H8Cl2O
SMILES:	CC(C)(Cl)C(=O)CCl
Mol. weight [g/mol]:	155.02

Physical Properties

Property code	Value	Unit	Source
gf	-158.72	kJ/mol	Joback Method
hf	-299.34	kJ/mol	Joback Method
hfus	11.29	kJ/mol	Joback Method
hvap	40.94	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.812		Crippen Method
mcvol	107.360	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpola	932.00		NIST Webbook
rinpola	932.00		NIST Webbook
tb	439.30	K	Joback Method
tc	645.91	K	Joback Method
tf	258.30	K	Joback Method
vc	0.408	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.93	J/molxK	439.30	Joback Method
cpg	232.16	J/molxK	611.47	Joback Method
cpg	225.21	J/molxK	577.04	Joback Method
cpg	217.75	J/molxK	542.60	Joback Method
cpg	209.74	J/molxK	508.17	Joback Method
cpg	201.14	J/molxK	473.73	Joback Method
cpg	238.61	J/molxK	645.91	Joback Method
dvisc	0.0004097	Paxs	439.30	Joback Method

dvisc	0.0005369	Paxs	409.13	Joback Method
dvisc	0.0007344	Paxs	378.97	Joback Method
dvisc	0.0010607	Paxs	348.80	Joback Method
dvisc	0.0016423	Paxs	318.63	Joback Method
dvisc	0.0027862	Paxs	288.47	Joback Method
dvisc	0.0053482	Paxs	258.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R629499&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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