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

Inchi: InChI=1S/C5H8Cl2O/c1-3(2)4(8)5(6)7/h3,5H,1-2H3
InchiKey: KVKWVIHYOWCBIK-UHFFFAOYSA-N
Formula: C5H8Cl2O
SMILES: CC(C)C(=O)C(Cl)Cl
Mol. weight [g/mol]: 155.02

Physical Properties

Property code	Value	Unit	Source
gf	-166.44	kJ/mol	Joback Method
hf	-301.15	kJ/mol	Joback Method
hfus	11.65	kJ/mol	Joback Method
hvap	41.46	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	2.015		Crippen Method
mcvol	107.360	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
rinpol	866.00		NIST Webbook
rinpol	866.00		NIST Webbook
tb	441.65	K	Joback Method
tc	644.37	K	Joback Method
tf	225.88	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.33	J/mol×K	441.65	Joback Method
cpg	198.04	J/mol×K	475.44	Joback Method
cpg	206.31	J/mol×K	509.22	Joback Method
cpg	214.14	J/mol×K	543.01	Joback Method
cpg	221.55	J/mol×K	576.80	Joback Method
cpg	228.55	J/mol×K	610.58	Joback Method
cpg	235.16	J/mol×K	644.37	Joback Method
dvisc	0.0082291	Pa×s	225.88	Joback Method

dvisc	0.0034166	Pa×s	261.84	Joback Method
dvisc	0.0017540	Pa×s	297.80	Joback Method
dvisc	0.0010396	Pa×s	333.76	Joback Method
dvisc	0.0006822	Pa×s	369.73	Joback Method
dvisc	0.0004824	Pa×s	405.69	Joback Method
dvisc	0.0003609	Pa×s	441.65	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=R629479&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