2-Butanone, 1,1-dichloro

Inchi: InChI=1S/C4H6Cl2O/c1-2-3(7)4(5)6/h4H,2H2,1H3
InchiKey: SNWBFNJXVNSVKM-UHFFFAOYSA-N
Formula: C4H6Cl2O
SMILES: CCC(=O)C(Cl)Cl
Mol. weight [g/mol]: 141.00

Physical Properties

Property code	Value	Unit	Source
gf	-172.42	kJ/mol	Joback Method
hf	-275.23	kJ/mol	Joback Method
hfus	12.59	kJ/mol	Joback Method
hvap	39.63	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.769		Crippen Method
mcvol	93.270	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	820.00		NIST Webbook
tb	419.21	K	Joback Method
tc	619.35	K	Joback Method
tf	229.61	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.85	J/mol×K	419.21	Joback Method
cpg	159.85	J/mol×K	452.57	Joback Method
cpg	166.50	J/mol×K	485.92	Joback Method
cpg	172.81	J/mol×K	519.28	Joback Method

cpg	178.78	J/mol×K	552.64	Joback Method
cpg	184.44	J/mol×K	585.99	Joback Method
cpg	189.78	J/mol×K	619.35	Joback Method
dvisc	0.0052966	Pa×s	229.61	Joback Method
dvisc	0.0026509	Pa×s	261.21	Joback Method
dvisc	0.0015405	Pa×s	292.81	Joback Method
dvisc	0.0009951	Pa×s	324.41	Joback Method
dvisc	0.0006946	Pa×s	356.01	Joback Method
dvisc	0.0005142	Pa×s	387.61	Joback Method
dvisc	0.0003982	Pa×s	419.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R629444&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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