methoxyacetyl chloride

Inchi: InChI=1S/C3H5ClO2/c1-6-2-3(4)5/h2H2,1H3
InchiKey: JJKWHOSQTYYFAE-UHFFFAOYSA-N
Formula: C3H5ClO2
SMILES: COCC(=O)Cl
Mol. weight [g/mol]: 108.52
CAS: 38870-89-2

Physical Properties

Property code	Value	Unit	Source
gf	-271.47	kJ/mol	Joback Method
hf	-365.79	kJ/mol	Joback Method
hfus	10.51	kJ/mol	Joback Method
hvap	35.81	kJ/mol	Joback Method
log10ws	-0.09		Crippen Method
logp	0.398		Crippen Method
mcvol	72.810	ml/mol	McGowan Method
pc	4462.28	kPa	Joback Method
tb	372.00 ± 10.00	K	NIST Webbook
tb	385.70	K	NIST Webbook
tb	386.00 ± 4.00	K	NIST Webbook
tb	386.00 ± 3.00	K	NIST Webbook
tb	372.00 ± 8.00	K	NIST Webbook
tc	570.48	K	Joback Method
tf	225.65	K	Joback Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.88	J/mol×K	381.76	Joback Method
cpg	123.10	J/mol×K	413.21	Joback Method
cpg	128.19	J/mol×K	444.67	Joback Method
cpg	133.14	J/mol×K	476.12	Joback Method
cpg	137.95	J/mol×K	507.57	Joback Method

cpg	142.60	J/mol×K	539.02	Joback Method
cpg	147.10	J/mol×K	570.48	Joback Method
dvisc	0.0025693	Pa×s	225.65	Joback Method
dvisc	0.0015292	Pa×s	251.67	Joback Method
dvisc	0.0010031	Pa×s	277.69	Joback Method
dvisc	0.0007073	Pa×s	303.70	Joback Method
dvisc	0.0005270	Pa×s	329.72	Joback Method
dvisc	0.0004099	Pa×s	355.74	Joback Method
dvisc	0.0003300	Pa×s	381.76	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38870892&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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