

4-(Chloroformyl)butyric acid, methyl ester

Other names:	methyl 4-chloroformylbutyrate
Inchi:	InChI=1S/C6H9ClO3/c1-10-6(9)4-2-3-5(7)8/h2-4H2,1H3
InchiKey:	JCAZSWWHFJVFPF-UHFFFAOYSA-N
Formula:	C6H9ClO3
SMILES:	COC(=O)CCCC(=O)Cl
Mol. weight [g/mol]:	164.59
CAS:	1501-26-4

Physical Properties

Property code	Value	Unit	Source
gf	-375.13	kJ/mol	Joback Method
hf	-540.29	kJ/mol	Joback Method
hfus	19.88	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.095		Crippen Method
mcvol	116.650	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
tb	504.27	K	Joback Method
tc	698.73	K	Joback Method
tf	309.39	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.35	J/mol×K	504.27	Joback Method
cpg	279.39	J/mol×K	666.32	Joback Method
cpg	271.94	J/mol×K	633.91	Joback Method
cpg	264.12	J/mol×K	601.50	Joback Method
cpg	255.91	J/mol×K	569.09	Joback Method
cpg	247.32	J/mol×K	536.68	Joback Method
cpg	286.45	J/mol×K	698.73	Joback Method
dvisc	0.0003287	Pa×s	504.27	Joback Method

dvisc	0.0004124	Pa×s	471.79	Joback Method
dvisc	0.0005350	Pa×s	439.31	Joback Method
dvisc	0.0007236	Pa×s	406.83	Joback Method
dvisc	0.0010312	Pa×s	374.35	Joback Method
dvisc	0.0015720	Pa×s	341.87	Joback Method
dvisc	0.0026181	Pa×s	309.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1501264&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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