Chloroacetic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C8H15ClO3/c1-7(3-4-11-2)6-12-8(10)5-9/h7H,3-6H2,1-2H3
InchiKey: IODHLYFOVDUSHK-UHFFFAOYSA-N
Formula: C8H15ClO3
SMILES: COCCC(C)COC(=O)CCl
Mol. weight [g/mol]: 194.66

Physical Properties

Property code	Value	Unit	Source
gf	-336.81	kJ/mol	Joback Method
hf	-606.49	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	48.97	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	1.441		Crippen Method
mcvol	149.130	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpol	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook
tb	518.14	K	Joback Method
tc	701.81	K	Joback Method
tf	289.23	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.74	J/mol×K	518.14	Joback Method
cpg	387.32	J/mol×K	671.20	Joback Method
cpg	377.12	J/mol×K	640.58	Joback Method
cpg	366.45	J/mol×K	609.97	Joback Method
cpg	355.33	J/mol×K	579.36	Joback Method
cpg	343.76	J/mol×K	548.75	Joback Method
cpg	397.07	J/mol×K	701.81	Joback Method
dvisc	0.0002013	Pa×s	518.14	Joback Method

dvisc	0.0002638	Pa×s	479.99	Joback Method
dvisc	0.0003623	Pa×s	441.84	Joback Method
dvisc	0.0005283	Pa×s	403.69	Joback Method
dvisc	0.0008334	Pa×s	365.53	Joback Method
dvisc	0.0014621	Pa×s	327.38	Joback Method
dvisc	0.0029751	Pa×s	289.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354608&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
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