Chloroacetic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C10H11ClO2/c1-7-3-8(2)5-9(4-7)13-10(12)6-11/h3-5H,6H2,1-2H3
InchiKey: WQVBITVXKZGBJJ-UHFFFAOYSA-N
Formula: C10H11ClO2
SMILES: Cc1cc(C)cc(OC(=O)CCl)c1
Mol. weight [g/mol]: 198.65

Physical Properties

Property code	Value	Unit	Source
gf	-119.38	kJ/mol	Joback Method
hf	-296.68	kJ/mol	Joback Method
hfus	21.90	kJ/mol	Joback Method
hvap	55.00	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.448		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1449.00		NIST Webbook
rinpol	1449.00		NIST Webbook
tb	578.56	K	Joback Method
tc	797.75	K	Joback Method
tf	356.00	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.21	J/mol×K	578.56	Joback Method
cpg	337.43	J/mol×K	615.09	Joback Method
cpg	348.97	J/mol×K	651.62	Joback Method
cpg	359.84	J/mol×K	688.16	Joback Method
cpg	370.04	J/mol×K	724.69	Joback Method
cpg	379.59	J/mol×K	761.22	Joback Method
cpg	388.49	J/mol×K	797.75	Joback Method
dvisc	0.0013217	Pa×s	356.00	Joback Method

dvisc	0.0008372	Pa×s	393.09	Joback Method
dvisc	0.0005738	Pa×s	430.19	Joback Method
dvisc	0.0004175	Pa×s	467.28	Joback Method
dvisc	0.0003184	Pa×s	504.37	Joback Method
dvisc	0.0002520	Pa×s	541.47	Joback Method
dvisc	0.0002055	Pa×s	578.56	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=U307713&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