2-Chloropropionic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C11H13ClO2/c1-7-4-8(2)6-10(5-7)14-11(13)9(3)12/h4-6,9H,1-3H3
InchiKey: SJELLOBJQJSXPZ-UHFFFAOYSA-N
Formula: C11H13ClO2
SMILES: Cc1cc(C)cc(OC(=O)C(C)Cl)c1
Mol. weight [g/mol]: 212.67

Physical Properties

Property code	Value	Unit	Source
gf	-113.40	kJ/mol	Joback Method
hf	-322.60	kJ/mol	Joback Method
hfus	20.97	kJ/mol	Joback Method
hvap	56.83	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.836		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1471.00		NIST Webbook
rinpol	1471.00		NIST Webbook
tb	601.00	K	Joback Method
tc	820.90	K	Joback Method
tf	352.27	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.53	J/mol×K	601.00	Joback Method
cpg	431.90	J/mol×K	784.25	Joback Method
cpg	421.53	J/mol×K	747.60	Joback Method
cpg	410.42	J/mol×K	710.95	Joback Method
cpg	398.56	J/mol×K	674.30	Joback Method
cpg	385.94	J/mol×K	637.65	Joback Method
cpg	441.54	J/mol×K	820.90	Joback Method
dvisc	0.0001757	Pa×s	601.00	Joback Method

dvisc	0.0002209	Pa×s	559.55	Joback Method
dvisc	0.0002880	Pa×s	518.09	Joback Method
dvisc	0.0003931	Pa×s	476.63	Joback Method
dvisc	0.0005695	Pa×s	435.18	Joback Method
dvisc	0.0008920	Pa×s	393.72	Joback Method
dvisc	0.0015527	Pa×s	352.27	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=U307753&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume