2,2-Dimethylpropanoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C13H18O2/c1-9-6-10(2)8-11(7-9)15-12(14)13(3,4)5/h6-8H,1-5H3
InchiKey: UHUMTAJLAWWWEZ-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: Cc1cc(C)cc(OC(=O)C(C)(C)C)c1
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	-79.35	kJ/mol	Joback Method
hf	-351.61	kJ/mol	Joback Method
hfus	18.06	kJ/mol	Joback Method
hvap	55.99	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.255		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
tb	606.54	K	Joback Method
tc	823.30	K	Joback Method
tf	362.31	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.89	J/mol×K	606.54	Joback Method
cpg	462.03	J/mol×K	642.67	Joback Method
cpg	477.18	J/mol×K	678.79	Joback Method
cpg	491.39	J/mol×K	714.92	Joback Method
cpg	504.69	J/mol×K	751.05	Joback Method
cpg	517.11	J/mol×K	787.17	Joback Method
cpg	528.68	J/mol×K	823.30	Joback Method
dvisc	0.0014420	Pa×s	362.31	Joback Method

dvisc	0.0008088	Pa×s	403.01	Joback Method
dvisc	0.0005044	Pa×s	443.72	Joback Method
dvisc	0.0003406	Pa×s	484.42	Joback Method
dvisc	0.0002444	Pa×s	525.13	Joback Method
dvisc	0.0001839	Pa×s	565.83	Joback Method
dvisc	0.0001438	Pa×s	606.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308041&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