2,2-Dimethylpropanoic acid, 3-methylphenyl ester

Inchi: InChI=1S/C12H16O2/c1-9-6-5-7-10(8-9)14-11(13)12(2,3)4/h5-8H,1-4H3
InchiKey: CHJUBXZEBVYVQV-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: Cc1cccc(OC(=O)C(C)(C)C)c1
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	-78.14	kJ/mol	Joback Method
hf	-319.50	kJ/mol	Joback Method
hfus	15.86	kJ/mol	Joback Method
hvap	53.10	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.947		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1315.00		NIST Webbook
tb	578.68	K	Joback Method
tc	798.32	K	Joback Method
tf	338.52	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.08	J/mol×K	578.68	Joback Method
cpg	412.88	J/mol×K	615.29	Joback Method
cpg	427.67	J/mol×K	651.89	Joback Method
cpg	441.50	J/mol×K	688.50	Joback Method
cpg	454.39	J/mol×K	725.10	Joback Method
cpg	466.41	J/mol×K	761.71	Joback Method
cpg	477.58	J/mol×K	798.32	Joback Method
dvisc	0.0019665	Pa×s	338.52	Joback Method
dvisc	0.0010426	Pa×s	378.55	Joback Method

dvisc	0.0006241	Pa×s	418.57	Joback Method
dvisc	0.0004086	Pa×s	458.60	Joback Method
dvisc	0.0002864	Pa×s	498.63	Joback Method
dvisc	0.0002116	Pa×s	538.65	Joback Method
dvisc	0.0001630	Pa×s	578.68	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=U308039&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