2-Methylpentanoic acid, 3,4-dimethylphenyl ester

Inchi: InChI=1S/C14H20O2/c1-5-6-11(3)14(15)16-13-8-7-10(2)12(4)9-13/h7-9,11H,5-6H2,1-4H

InchiKey: GEBCPKNJBOHNGU-UHFFFAOYSA-N

Formula: C14H20O2

SMILES: CCCC(C)C(=O)Oc1ccc(C)c(C)c1

Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
gf	-76.21	kJ/mol	Joback Method
hf	-368.78	kJ/mol	Joback Method
hfus	24.54	kJ/mol	Joback Method
hvap	59.13	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.645		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1652.00		NIST Webbook
tb	632.21	K	Joback Method
tc	837.91	K	Joback Method
tf	356.16	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.94	J/mol×K	632.21	Joback Method
cpg	566.69	J/mol×K	803.63	Joback Method
cpg	553.84	J/mol×K	769.34	Joback Method
cpg	540.15	J/mol×K	735.06	Joback Method
cpg	525.62	J/mol×K	700.78	Joback Method
cpg	510.22	J/mol×K	666.49	Joback Method
cpg	578.72	J/mol×K	837.91	Joback Method
dvisc	0.0001377	Pa×s	632.21	Joback Method
dvisc	0.0001757	Pa×s	586.20	Joback Method

dvisc	0.0002338	Pa×s	540.19	Joback Method
dvisc	0.0003281	Pa×s	494.19	Joback Method
dvisc	0.0004935	Pa×s	448.18	Joback Method
dvisc	0.0008151	Pa×s	402.17	Joback Method
dvisc	0.0015325	Pa×s	356.16	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=U357383&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