2-Methylpropionic acid, 3-methylphenyl ester

Inchi: InChI=1S/C11H14O2/c1-8(2)11(12)13-10-6-4-5-9(3)7-10/h4-8H,1-3H3
InchiKey: CGXNGUPLQGZMAC-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: Cc1cccc(OC(=O)C(C)C)c1
Mol. weight [g/mol]: 178.23

Physical Properties

Property code	Value	Unit	Source
gf	-91.84	kJ/mol	Joback Method
hf	-295.39	kJ/mol	Joback Method
hfus	17.16	kJ/mol	Joback Method
hvap	51.79	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.556		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	1288.00		NIST Webbook
tb	558.59	K	Joback Method
tc	773.47	K	Joback Method
tf	309.83	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.51	J/mol×K	558.59	Joback Method
cpg	361.03	J/mol×K	594.40	Joback Method
cpg	374.76	J/mol×K	630.22	Joback Method
cpg	387.70	J/mol×K	666.03	Joback Method
cpg	399.87	J/mol×K	701.84	Joback Method
cpg	411.28	J/mol×K	737.66	Joback Method
cpg	421.95	J/mol×K	773.47	Joback Method
dvisc	0.0022187	Pa×s	309.83	Joback Method
dvisc	0.0011460	Pa×s	351.29	Joback Method

dvisc	0.0006805	Pa×s	392.75	Joback Method
dvisc	0.0004464	Pa×s	434.21	Joback Method
dvisc	0.0003151	Pa×s	475.67	Joback Method
dvisc	0.0002352	Pa×s	517.13	Joback Method
dvisc	0.0001834	Pa×s	558.59	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=U308014&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