2,2-Dimethylpropanoic acid, 2-naphthyl ester

Inchi: InChI=1S/C15H16O2/c1-15(2,3)14(16)17-13-9-8-11-6-4-5-7-12(11)10-13/h4-10H,1-3H3
InchiKey: SUGMMMOSTHSMJT-UHFFFAOYSA-N
Formula: C15H16O2
SMILES: CC(C)(C)C(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 228.29

Physical Properties

Property code	Value	Unit	Source
gf	53.77	kJ/mol	Joback Method
hf	-190.35	kJ/mol	Joback Method
hfus	20.65	kJ/mol	Joback Method
hvap	61.42	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.791		Crippen Method
mcvol	186.430	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1756.00		NIST Webbook
tb	666.30	K	Joback Method
tc	901.26	K	Joback Method
tf	405.03	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.87	J/mol×K	666.30	Joback Method
cpg	503.59	J/mol×K	705.46	Joback Method
cpg	518.11	J/mol×K	744.62	Joback Method
cpg	531.52	J/mol×K	783.78	Joback Method
cpg	543.92	J/mol×K	822.94	Joback Method
cpg	555.40	J/mol×K	862.10	Joback Method
cpg	566.05	J/mol×K	901.26	Joback Method
dvisc	0.0014197	Pa×s	405.03	Joback Method
dvisc	0.0008756	Pa×s	448.57	Joback Method

dvisc	0.0005883	Pa×s	492.12	Joback Method
dvisc	0.0004216	Pa×s	535.66	Joback Method
dvisc	0.0003177	Pa×s	579.21	Joback Method
dvisc	0.0002491	Pa×s	622.75	Joback Method
dvisc	0.0002016	Pa×s	666.30	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=U308046&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