1-Naphthoic acid, 2-methylpentyl ester

Inchi: InChI=1S/C17H20O2/c1-3-7-13(2)12-19-17(18)16-11-6-9-14-8-4-5-10-15(14)16/h4-6,8-1
InchiKey: IQBIVYNIHNPLJH-UHFFFAOYSA-N
Formula: C17H20O2
SMILES: CCCC(C)COC(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	65.33	kJ/mol	Joback Method
hf	-228.16	kJ/mol	Joback Method
hfus	29.72	kJ/mol	Joback Method
hvap	66.78	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.433		Crippen Method
mcvol	214.610	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2129.00		NIST Webbook
rinpol	2129.00		NIST Webbook
tb	714.85	K	Joback Method
tc	933.61	K	Joback Method
tf	410.15	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.06	J/mol×K	714.85	Joback Method
cpg	661.85	J/mol×K	897.15	Joback Method
cpg	649.60	J/mol×K	860.69	Joback Method
cpg	636.46	J/mol×K	824.23	Joback Method
cpg	622.36	J/mol×K	787.77	Joback Method
cpg	607.25	J/mol×K	751.31	Joback Method
cpg	673.26	J/mol×K	933.61	Joback Method
dvisc	0.0001810	Pa×s	714.85	Joback Method

dvisc	0.0002242	Pa×s	664.07	Joback Method
dvisc	0.0002878	Pa×s	613.28	Joback Method
dvisc	0.0003864	Pa×s	562.50	Joback Method
dvisc	0.0005501	Pa×s	511.72	Joback Method
dvisc	0.0008465	Pa×s	460.93	Joback Method
dvisc	0.0014493	Pa×s	410.15	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=U355688&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