1-Naphthoic acid, 3-methylbutyl ester

Inchi: InChI=1S/C16H18O2/c1-12(2)10-11-18-16(17)15-9-5-7-13-6-3-4-8-14(13)15/h3-9,12H,1
InchiKey: GJIJYBQGGMJLCH-UHFFFAOYSA-N
Formula: C16H18O2
SMILES: CC(C)CCOC(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	56.91	kJ/mol	Joback Method
hf	-207.52	kJ/mol	Joback Method
hfus	27.13	kJ/mol	Joback Method
hvap	64.56	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.043		Crippen Method
mcvol	200.520	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	691.97	K	Joback Method
tc	914.36	K	Joback Method
tf	398.88	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.59	J/mol×K	691.97	Joback Method
cpg	553.44	J/mol×K	729.03	Joback Method
cpg	568.21	J/mol×K	766.10	Joback Method
cpg	581.97	J/mol×K	803.16	Joback Method
cpg	594.78	J/mol×K	840.23	Joback Method
cpg	606.69	J/mol×K	877.29	Joback Method
cpg	617.76	J/mol×K	914.36	Joback Method
dvisc	0.0015154	Pa×s	398.88	Joback Method

dvisc	0.0008993	Pa×s	447.73	Joback Method
dvisc	0.0005914	Pa×s	496.58	Joback Method
dvisc	0.0004192	Pa×s	545.42	Joback Method
dvisc	0.0003145	Pa×s	594.27	Joback Method
dvisc	0.0002464	Pa×s	643.12	Joback Method
dvisc	0.0001999	Pa×s	691.97	Joback Method

Sources

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=U355686&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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