1-Naphthoic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C17H20O3/c1-13(10-11-19-2)12-20-17(18)16-9-5-7-14-6-3-4-8-15(14)16/h3-9,

InchiKey: UICKNFHOMVIQLO-UHFFFAOYSA-N

Formula: C17H20O3

SMILES: COCCC(C)COC(=O)c1cccc2ccccc12

Mol. weight [g/mol]: 272.34

Physical Properties

Property code	Value	Unit	Source
gf	-39.67	kJ/mol	Joback Method
hf	-360.38	kJ/mol	Joback Method
hfus	30.91	kJ/mol	Joback Method
hvap	69.19	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.669		Crippen Method
mcvol	220.480	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2259.00		NIST Webbook
tb	737.27	K	Joback Method
tc	953.78	K	Joback Method
tf	432.38	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.42	J/mol×K	737.27	Joback Method
cpg	687.00	J/mol×K	917.69	Joback Method
cpg	675.24	J/mol×K	881.61	Joback Method
cpg	662.54	J/mol×K	845.52	Joback Method
cpg	648.87	J/mol×K	809.44	Joback Method
cpg	634.18	J/mol×K	773.35	Joback Method
cpg	697.88	J/mol×K	953.78	Joback Method
dvisc	0.0001417	Pa×s	737.27	Joback Method
dvisc	0.0001753	Pa×s	686.45	Joback Method

dvisc	0.0002245	Pa×s	635.64	Joback Method
dvisc	0.0003002	Pa×s	584.83	Joback Method
dvisc	0.0004241	Pa×s	534.01	Joback Method
dvisc	0.0006443	Pa×s	483.19	Joback Method
dvisc	0.0010801	Pa×s	432.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355690&Units=SI
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

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