1-Naphthaleneacetic acid, 3-methylbut-2-yl ester

Inchi: InChI=1S/C17H20O2/c1-12(2)13(3)19-17(18)11-15-9-6-8-14-7-4-5-10-16(14)15/h4-10,12

InchiKey: CDIGFHPWOZKBCI-UHFFFAOYSA-N

Formula: C17H20O2

SMILES: CC(C)C(C)OC(=O)Cc1cccc2ccccc12

Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	62.89	kJ/mol	Joback Method
hf	-233.44	kJ/mol	Joback Method
hfus	26.20	kJ/mol	Joback Method
hvap	66.39	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.970		Crippen Method
mcvol	214.610	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	2476.00		NIST Webbook
rinpol	2476.00		NIST Webbook
tb	714.41	K	Joback Method
tc	937.14	K	Joback Method
tf	395.15	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.58	J/mol×K	714.41	Joback Method
cpg	608.09	J/mol×K	751.53	Joback Method
cpg	623.47	J/mol×K	788.65	Joback Method
cpg	637.78	J/mol×K	825.77	Joback Method
cpg	651.09	J/mol×K	862.90	Joback Method
cpg	663.46	J/mol×K	900.02	Joback Method
cpg	674.96	J/mol×K	937.14	Joback Method
dvisc	0.0016788	Pa×s	395.15	Joback Method

dvisc	0.0009098	Pa×s	448.36	Joback Method
dvisc	0.0005615	Pa×s	501.57	Joback Method
dvisc	0.0003802	Pa×s	554.78	Joback Method
dvisc	0.0002756	Pa×s	607.99	Joback Method
dvisc	0.0002104	Pa×s	661.20	Joback Method
dvisc	0.0001672	Pa×s	714.41	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=U415044&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