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

Inchi: InChI=1S/C18H22O2/c1-4-17(13(2)3)20-18(19)12-15-10-7-9-14-8-5-6-11-16(14)15/h5-11

InchiKey: MCKBYDBUXYJHRK-UHFFFAOYSA-N

Formula: C18H22O2

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

Mol. weight [g/mol]: 270.37

Physical Properties

Property code	Value	Unit	Source
gf	71.31	kJ/mol	Joback Method
hf	-254.08	kJ/mol	Joback Method
hfus	28.79	kJ/mol	Joback Method
hvap	68.62	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.360		Crippen Method
mcvol	228.700	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook
tb	737.29	K	Joback Method
tc	956.53	K	Joback Method
tf	406.42	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.23	J/mol×K	737.29	Joback Method
cpg	663.00	J/mol×K	773.83	Joback Method
cpg	678.65	J/mol×K	810.37	Joback Method
cpg	693.24	J/mol×K	846.91	Joback Method
cpg	706.82	J/mol×K	883.45	Joback Method
cpg	719.47	J/mol×K	919.99	Joback Method
cpg	731.25	J/mol×K	956.53	Joback Method
dvisc	0.0015855	Pa×s	406.42	Joback Method

dvisc	0.0008467	Pa×s	461.56	Joback Method
dvisc	0.0005170	Pa×s	516.71	Joback Method
dvisc	0.0003471	Pa×s	571.86	Joback Method
dvisc	0.0002500	Pa×s	627.00	Joback Method
dvisc	0.0001899	Pa×s	682.14	Joback Method
dvisc	0.0001503	Pa×s	737.29	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=U415045&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

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