

1-Naphthoic acid, oct-3-en-2-yl ester

Inchi:	InChI=1S/C19H22O2/c1-3-4-5-6-10-15(2)21-19(20)18-14-9-12-16-11-7-8-13-17(16)18/h6
InchiKey:	LNTUTQXSICAIDV-UXBLZVDNSA-N
Formula:	C19H22O2
SMILES:	CCCCC=CC(C)OC(=O)c1cccc2ccccc12
Mol. weight [g/mol]:	282.38

Physical Properties

Property code	Value	Unit	Source
gf	162.39	kJ/mol	Joback Method
hf	-152.22	kJ/mol	Joback Method
hfus	35.10	kJ/mol	Joback Method
hvap	71.19	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.131		Crippen Method
mcvol	238.490	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinsol	2192.00		NIST Webbook
tb	764.77	K	Joback Method
tc	984.66	K	Joback Method
tf	427.61	K	Joback Method
vc	0.911	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.75	J/molxK	764.77	Joback Method
cpg	693.00	J/molxK	801.42	Joback Method
cpg	708.19	J/molxK	838.07	Joback Method
cpg	722.39	J/molxK	874.71	Joback Method
cpg	735.70	J/molxK	911.36	Joback Method
cpg	748.20	J/molxK	948.01	Joback Method
cpg	759.96	J/molxK	984.66	Joback Method
dvisc	0.0011846	Paxs	427.61	Joback Method
dvisc	0.0006576	Paxs	483.80	Joback Method

dvisc	0.0004127	Paxs	540.00	Joback Method
dvisc	0.0002827	Paxs	596.19	Joback Method
dvisc	0.0002068	Paxs	652.38	Joback Method
dvisc	0.0001589	Paxs	708.58	Joback Method
dvisc	0.0001269	Paxs	764.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U308822&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

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