1-Naphthoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C21H22O2/c1-15(2)12-13-18(14-16(3)4)23-21(22)20-11-7-9-17-8-5-6-10-19(17

InchiKey: YWDNWKDCBRGVGC-UHFFFAOYSA-N

Formula: C21H22O2

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)c1cccc2ccccc12

Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	378.66	kJ/mol	Joback Method
hf	71.94	kJ/mol	Joback Method
hfus	37.09	kJ/mol	Joback Method
hvap	76.86	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	4.991		Crippen Method
mcvol	258.070	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	2277.00		NIST Webbook
tb	811.49	K	Joback Method
tc	1048.16	K	Joback Method
tf	530.61	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.38	J/mol×K	811.49	Joback Method
cpg	756.04	J/mol×K	850.93	Joback Method
cpg	771.52	J/mol×K	890.38	Joback Method
cpg	785.90	J/mol×K	929.82	Joback Method
cpg	799.29	J/mol×K	969.27	Joback Method
cpg	811.76	J/mol×K	1008.71	Joback Method
cpg	823.43	J/mol×K	1048.16	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=U308824&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
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