1-Naphthoic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C22H24O2/c1-5-9-17(4)21(15-14-16(2)3)24-22(23)20-13-8-11-18-10-6-7-12-19

InchiKey: ZADXSOUCXHUWLU-UHFFFAOYSA-N

Formula: C22H24O2

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

Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	387.08	kJ/mol	Joback Method
hf	51.30	kJ/mol	Joback Method
hfus	39.68	kJ/mol	Joback Method
hvap	79.09	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	5.381		Crippen Method
mcvol	272.160	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	834.37	K	Joback Method
tc	1067.45	K	Joback Method
tf	541.88	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.59	J/mol×K	834.37	Joback Method
cpg	813.42	J/mol×K	873.22	Joback Method
cpg	829.07	J/mol×K	912.06	Joback Method
cpg	843.65	J/mol×K	950.91	Joback Method
cpg	857.24	J/mol×K	989.75	Joback Method
cpg	869.94	J/mol×K	1028.60	Joback Method
cpg	881.85	J/mol×K	1067.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308825&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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