1-Naphthoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C17H16O2/c1-3-8-14(4-2)19-17(18)16-12-7-10-13-9-5-6-11-15(13)16/h5-7,9-1
InchiKey: FXZIUEILTHGESM-UHFFFAOYSA-N
Formula: C17H16O2
SMILES: CC#CC(CC)OC(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 252.31

Physical Properties

Property code	Value	Unit	Source
gf	268.13	kJ/mol	Joback Method
hf	44.14	kJ/mol	Joback Method
hfus	32.84	kJ/mol	Joback Method
hvap	68.93	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	3.798		Crippen Method
mcvol	206.010	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	2040.00		NIST Webbook
tb	723.85	K	Joback Method
tc	966.09	K	Joback Method
tf	516.25	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.59	J/mol×K	723.85	Joback Method
cpg	560.23	J/mol×K	764.22	Joback Method
cpg	574.72	J/mol×K	804.60	Joback Method
cpg	588.14	J/mol×K	844.97	Joback Method
cpg	600.55	J/mol×K	885.34	Joback Method
cpg	612.02	J/mol×K	925.72	Joback Method
cpg	622.65	J/mol×K	966.09	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=U308821&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