1-Naphthoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C16H12O2/c1-2-3-6-12-18-16(17)15-11-7-9-13-8-4-5-10-14(13)15/h1,3-11H,12
InchiKey: GFQDQLYAGSQRIW-UHFFFAOYSA-N
Formula: C16H12O2
SMILES: C#CC=CCOC(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 236.27

Physical Properties

Property code	Value	Unit	Source
gf	362.64	kJ/mol	Joback Method
hf	206.88	kJ/mol	Joback Method
hfus	33.83	kJ/mol	Joback Method
hvap	64.76	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	3.186		Crippen Method
mcvol	187.620	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	2016.00		NIST Webbook
tb	686.69	K	Joback Method
tc	928.56	K	Joback Method
tf	455.77	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.08	J/mol×K	686.69	Joback Method
cpg	480.86	J/mol×K	727.00	Joback Method
cpg	493.59	J/mol×K	767.31	Joback Method
cpg	505.36	J/mol×K	807.62	Joback Method
cpg	516.29	J/mol×K	847.94	Joback Method
cpg	526.48	J/mol×K	888.25	Joback Method
cpg	536.03	J/mol×K	928.56	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=U308820&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