1-Naphthaleneacetic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C16H14O2/c1-3-12(2)18-16(17)11-14-9-6-8-13-7-4-5-10-15(13)14/h1,4-10,12H
InchiKey: RSKPBRCHCWXUPN-UHFFFAOYSA-N
Formula: C16H14O2
SMILES: C#CC(C)OC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]: 238.28

Physical Properties

Property code	Value	Unit	Source
gf	279.98	kJ/mol	Joback Method
hf	84.38	kJ/mol	Joback Method
hfus	30.11	kJ/mol	Joback Method
hvap	64.41	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	2.947		Crippen Method
mcvol	191.920	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook
tb	682.09	K	Joback Method
tc	919.12	K	Joback Method
tf	445.85	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.63	J/mol×K	682.09	Joback Method
cpg	505.38	J/mol×K	721.59	Joback Method
cpg	519.04	J/mol×K	761.10	Joback Method
cpg	531.69	J/mol×K	800.60	Joback Method
cpg	543.39	J/mol×K	840.11	Joback Method
cpg	554.23	J/mol×K	879.61	Joback Method
cpg	564.30	J/mol×K	919.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415043&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

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