1-Naphthoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C18H11NO2/c19-12-13-8-10-15(11-9-13)21-18(20)17-7-3-5-14-4-1-2-6-16(14)
InchiKey: XJZYDLZARKPZFG-UHFFFAOYSA-N
Formula: C18H11NO2
SMILES: N#Cc1ccc(OC(=O)c2cccc3ccccc23)cc1
Mol. weight [g/mol]: 273.29

Physical Properties

Property code	Value	Unit	Source
gf	312.15	kJ/mol	Joback Method
hf	146.42	kJ/mol	Joback Method
hfus	30.99	kJ/mol	Joback Method
hvap	82.81	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	3.931		Crippen Method
mcvol	206.320	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	2542.00		NIST Webbook
rinpol	2542.00		NIST Webbook
tb	871.91	K	Joback Method
tc	1132.38	K	Joback Method
tf	540.35	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.09	J/mol×K	871.91	Joback Method
cpg	579.20	J/mol×K	915.32	Joback Method
cpg	589.30	J/mol×K	958.73	Joback Method
cpg	598.48	J/mol×K	1002.15	Joback Method
cpg	606.87	J/mol×K	1045.56	Joback Method
cpg	614.56	J/mol×K	1088.97	Joback Method
cpg	621.65	J/mol×K	1132.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307827&Units=SI

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