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

Inchi: InChI=1S/C19H21NO2/c1-5-6-15(4)18(12-7-14(2)3)22-19(21)17-10-8-16(13-20)9-11-17/h
InchiKey: ARBGFWDAVXOGHV-UHFFFAOYSA-N
Formula: C19H21NO2
SMILES: C=C(C)C#CC(OC(=O)c1ccc(C#N)cc1)C(C)CCC
Mol. weight [g/mol]: 295.38

Physical Properties

Property code	Value	Unit	Source
gf	388.35	kJ/mol	Joback Method
hf	87.03	kJ/mol	Joback Method
hfus	36.40	kJ/mol	Joback Method
hvap	81.25	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.099		Crippen Method
mcvol	250.730	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	2084.00		NIST Webbook
tb	848.83	K	Joback Method
tc	1080.56	K	Joback Method
tf	540.36	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.19	J/mol×K	848.83	Joback Method
cpg	737.54	J/mol×K	887.45	Joback Method
cpg	750.77	J/mol×K	926.07	Joback Method
cpg	762.93	J/mol×K	964.69	Joback Method
cpg	774.08	J/mol×K	1003.32	Joback Method
cpg	784.26	J/mol×K	1041.94	Joback Method
cpg	793.53	J/mol×K	1080.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299228&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