4-Cyanobenzoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C14H13NO2/c1-3-5-13(4-2)17-14(16)12-8-6-11(10-15)7-9-12/h6-9,13H,4H2,1-
InchiKey: GTIHYBGVDHCOHP-UHFFFAOYSA-N
Formula: C14H13NO2
SMILES: CC#CC(CC)OC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 227.26

Physical Properties

Property code	Value	Unit	Source
gf	269.40	kJ/mol	Joback Method
hf	79.87	kJ/mol	Joback Method
hfus	29.56	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.517		Crippen Method
mcvol	184.580	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1754.00		NIST Webbook
rinpol	1754.00		NIST Webbook
tb	738.31	K	Joback Method
tc	978.28	K	Joback Method
tf	514.73	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.52	J/mol×K	738.31	Joback Method
cpg	489.32	J/mol×K	778.30	Joback Method
cpg	501.16	J/mol×K	818.30	Joback Method
cpg	512.05	J/mol×K	858.29	Joback Method
cpg	522.03	J/mol×K	898.29	Joback Method
cpg	531.12	J/mol×K	938.28	Joback Method
cpg	539.34	J/mol×K	978.28	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=U299224&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

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