4-Cyanobenzoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C13H9NO2/c1-2-3-4-9-16-13(15)12-7-5-11(10-14)6-8-12/h1,3-8H,9H2/b4-3-
InchiKey: VUYBUXDCYOZSDM-ARJAWSKDSA-N
Formula: C13H9NO2
SMILES: C#CC=CCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 211.22

Physical Properties

Property code	Value	Unit	Source
gf	363.91	kJ/mol	Joback Method
hf	242.61	kJ/mol	Joback Method
hfus	30.55	kJ/mol	Joback Method
hvap	66.92	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	1.904		Crippen Method
mcvol	166.190	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	701.15	K	Joback Method
tc	940.69	K	Joback Method
tf	454.25	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.62	J/mol×K	701.15	Joback Method
cpg	411.44	J/mol×K	741.07	Joback Method
cpg	421.44	J/mol×K	781.00	Joback Method
cpg	430.69	J/mol×K	820.92	Joback Method
cpg	439.22	J/mol×K	860.84	Joback Method
cpg	447.10	J/mol×K	900.77	Joback Method
cpg	454.37	J/mol×K	940.69	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=U299223&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