4-Cyanobenzoic acid, 3-methyl-2-enyl ester

Inchi: InChI=1S/C13H13NO2/c1-10(2)7-8-16-13(15)12-5-3-11(9-14)4-6-12/h3-7H,8H2,1-2H3
InchiKey: DLINGEMBUUQSLN-UHFFFAOYSA-N
Formula: C13H13NO2
SMILES: CC(C)=CCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 215.25

Physical Properties

Property code	Value	Unit	Source
gf	132.29	kJ/mol	Joback Method
hf	-59.08	kJ/mol	Joback Method
hfus	26.26	kJ/mol	Joback Method
hvap	67.14	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.681		Crippen Method
mcvol	174.790	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1706.00		NIST Webbook
tb	710.91	K	Joback Method
tc	939.39	K	Joback Method
tf	393.32	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.41	J/mol×K	710.91	Joback Method
cpg	459.76	J/mol×K	748.99	Joback Method
cpg	471.25	J/mol×K	787.07	Joback Method
cpg	481.93	J/mol×K	825.15	Joback Method
cpg	491.82	J/mol×K	863.23	Joback Method
cpg	500.99	J/mol×K	901.31	Joback Method
cpg	509.45	J/mol×K	939.39	Joback Method

Sources

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=U299222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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