4-Cyanobenzoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C16H19NO2/c1-3-4-5-6-7-13(2)19-16(18)15-10-8-14(12-17)9-11-15/h6-11,13H
InchiKey: NLWBQHCRUYYUFT-VOTSOKGWSA-N
Formula: C16H19NO2
SMILES: CCCCC=CC(C)OC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 257.33

Physical Properties

Property code	Value	Unit	Source
gf	163.66	kJ/mol	Joback Method
hf	-116.49	kJ/mol	Joback Method
hfus	31.82	kJ/mol	Joback Method
hvap	73.35	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.850		Crippen Method
mcvol	217.060	ml/mol	McGowan Method
pc	1800.03	kPa	Joback Method
rinpol	1915.00		NIST Webbook
rinpol	1915.00		NIST Webbook
tb	779.23	K	Joback Method
tc	997.91	K	Joback Method
tf	426.09	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.15	J/mol×K	779.23	Joback Method
cpg	620.94	J/mol×K	815.68	Joback Method
cpg	633.78	J/mol×K	852.12	Joback Method
cpg	645.72	J/mol×K	888.57	Joback Method
cpg	656.82	J/mol×K	925.02	Joback Method
cpg	667.11	J/mol×K	961.47	Joback Method
cpg	676.65	J/mol×K	997.91	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=U299225&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