4-Cyanobenzoic acid, undec-2-enyl ester

Inchi: InChI=1S/C19H25NO2/c1-2-3-4-5-6-7-8-9-10-15-22-19(21)18-13-11-17(16-20)12-14-18/h
InchiKey: BTNFTBZJFUVRKM-MDZDMXLPSA-N
Formula: C19H25NO2
SMILES: CCCCCCCCC=CCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 299.41

Physical Properties

Property code	Value	Unit	Source
gf	191.36	kJ/mol	Joback Method
hf	-173.13	kJ/mol	Joback Method
hfus	43.11	kJ/mol	Joback Method
hvap	80.42	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.022		Crippen Method
mcvol	259.330	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
tb	848.31	K	Joback Method
tc	1059.02	K	Joback Method
tf	474.90	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.14	J/mol×K	848.31	Joback Method
cpg	789.68	J/mol×K	883.43	Joback Method
cpg	803.27	J/mol×K	918.55	Joback Method
cpg	815.96	J/mol×K	953.67	Joback Method
cpg	827.80	J/mol×K	988.79	Joback Method
cpg	838.83	J/mol×K	1023.90	Joback Method
cpg	849.12	J/mol×K	1059.02	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=U299229&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