4-Cyanobenzoic acid, nonyl ester

Inchi: InChI=1S/C17H23NO2/c1-2-3-4-5-6-7-8-13-20-17(19)16-11-9-15(14-18)10-12-16/h9-12H
InchiKey: DRVHHMDHRUJORH-UHFFFAOYSA-N
Formula: C17H23NO2
SMILES: CCCCCCCCCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 273.37

Physical Properties

Property code	Value	Unit	Source
gf	94.30	kJ/mol	Joback Method
hf	-249.07	kJ/mol	Joback Method
hfus	37.73	kJ/mol	Joback Method
hvap	76.01	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.466		Crippen Method
mcvol	235.450	ml/mol	McGowan Method
pc	1583.49	kPa	Joback Method
rinpol	2142.10		NIST Webbook
rinpol	2142.10		NIST Webbook
tb	798.39	K	Joback Method
tc	1005.68	K	Joback Method
tf	457.44	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.59	J/mol×K	798.39	Joback Method
cpg	702.02	J/mol×K	832.94	Joback Method
cpg	715.48	J/mol×K	867.49	Joback Method
cpg	728.02	J/mol×K	902.03	Joback Method
cpg	739.67	J/mol×K	936.58	Joback Method
cpg	750.44	J/mol×K	971.13	Joback Method
cpg	760.38	J/mol×K	1005.68	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=U292448&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