4-Cyanobenzoic acid, undecyl ester

Inchi: InChI=1S/C19H27NO2/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: CERKUVNHDXVIQZ-UHFFFAOYSA-N
Formula: C19H27NO2
SMILES: CCCCCCCCCCCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 301.42

Physical Properties

Property code	Value	Unit	Source
gf	111.14	kJ/mol	Joback Method
hf	-290.35	kJ/mol	Joback Method
hfus	42.91	kJ/mol	Joback Method
hvap	80.46	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.246		Crippen Method
mcvol	263.630	ml/mol	McGowan Method
pc	1366.68	kPa	Joback Method
rinpol	2313.30		NIST Webbook
tb	844.15	K	Joback Method
tc	1050.07	K	Joback Method
tf	479.98	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.85	J/mol×K	844.15	Joback Method
cpg	816.83	J/mol×K	878.47	Joback Method
cpg	830.81	J/mol×K	912.79	Joback Method
cpg	843.80	J/mol×K	947.11	Joback Method
cpg	855.85	J/mol×K	981.43	Joback Method
cpg	866.99	J/mol×K	1015.75	Joback Method
cpg	877.26	J/mol×K	1050.07	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=U292452&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