4-Cyanobenzoic acid, octyl ester

Inchi: InChI=1S/C16H21NO2/c1-2-3-4-5-6-7-12-19-16(18)15-10-8-14(13-17)9-11-15/h8-11H,2-
InchiKey: SKJQGJGHSZPIFH-UHFFFAOYSA-N
Formula: C16H21NO2
SMILES: CCCCCCCCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 259.34

Physical Properties

Property code	Value	Unit	Source
gf	85.88	kJ/mol	Joback Method
hf	-228.43	kJ/mol	Joback Method
hfus	35.14	kJ/mol	Joback Method
hvap	73.78	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.076		Crippen Method
mcvol	221.360	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook
tb	775.51	K	Joback Method
tc	984.39	K	Joback Method
tf	446.17	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.90	J/mol×K	775.51	Joback Method
cpg	646.00	J/mol×K	810.32	Joback Method
cpg	659.17	J/mol×K	845.14	Joback Method
cpg	671.44	J/mol×K	879.95	Joback Method
cpg	682.84	J/mol×K	914.77	Joback Method
cpg	693.38	J/mol×K	949.58	Joback Method
cpg	703.11	J/mol×K	984.39	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=U299833&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