4-Cyanobenzoic acid, decyl ester

Inchi: InChI=1S/C18H25NO2/c1-2-3-4-5-6-7-8-9-14-21-18(20)17-12-10-16(15-19)11-13-17/h10
InchiKey: DNLLYQQKAAVLPE-UHFFFAOYSA-N
Formula: C18H25NO2
SMILES: CCCCCCCCCCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 287.40

Physical Properties

Property code	Value	Unit	Source
gf	102.72	kJ/mol	Joback Method
hf	-269.71	kJ/mol	Joback Method
hfus	40.32	kJ/mol	Joback Method
hvap	78.23	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.856		Crippen Method
mcvol	249.540	ml/mol	McGowan Method
pc	1469.10	kPa	Joback Method
rinpol	2220.00		NIST Webbook
tb	821.27	K	Joback Method
tc	1027.55	K	Joback Method
tf	468.71	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.27	J/mol×K	821.27	Joback Method
cpg	758.98	J/mol×K	855.65	Joback Method
cpg	772.71	J/mol×K	890.03	Joback Method
cpg	785.49	J/mol×K	924.41	Joback Method
cpg	797.35	J/mol×K	958.79	Joback Method
cpg	808.32	J/mol×K	993.17	Joback Method
cpg	818.44	J/mol×K	1027.55	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=U299834&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