4-Cyanobenzoic acid, pentadecyl ester

Inchi: InChI=1S/C23H35NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-19-26-23(25)22-17-15-21(20-
InchiKey: WXVFKSKXNUHSII-UHFFFAOYSA-N
Formula: C23H35NO2
SMILES: CCCCCCCCCCCCCCCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 357.53

Physical Properties

Property code	Value	Unit	Source
gf	144.82	kJ/mol	Joback Method
hf	-372.91	kJ/mol	Joback Method
hfus	53.27	kJ/mol	Joback Method
hvap	89.36	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	6.806		Crippen Method
mcvol	319.990	ml/mol	McGowan Method
pc	1048.01	kPa	Joback Method
rinpol	2740.00		NIST Webbook
tb	935.67	K	Joback Method
tc	1147.55	K	Joback Method
tf	525.06	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.98	J/mol×K	935.67	Joback Method
cpg	1056.04	J/mol×K	970.98	Joback Method
cpg	1070.93	J/mol×K	1006.30	Joback Method
cpg	1084.69	J/mol×K	1041.61	Joback Method
cpg	1097.40	J/mol×K	1076.92	Joback Method
cpg	1109.08	J/mol×K	1112.24	Joback Method
cpg	1119.80	J/mol×K	1147.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299839&Units=SI
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

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