4-Cyanobenzoic acid, tetradecyl ester

Inchi: InChI=1S/C22H33NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-25-22(24)21-16-14-20(19-23)
InchiKey: GHWJYNVUWQLING-UHFFFAOYSA-N
Formula: C22H33NO2
SMILES: CCCCCCCCCCCCCCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 343.50

Physical Properties

Property code	Value	Unit	Source
gf	136.40	kJ/mol	Joback Method
hf	-352.27	kJ/mol	Joback Method
hfus	50.68	kJ/mol	Joback Method
hvap	87.14	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	6.416		Crippen Method
mcvol	305.900	ml/mol	McGowan Method
pc	1116.31	kPa	Joback Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook
tb	912.79	K	Joback Method
tc	1121.96	K	Joback Method
tf	513.79	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	979.40	J/mol×K	912.79	Joback Method
cpg	995.17	J/mol×K	947.65	Joback Method
cpg	1009.82	J/mol×K	982.51	Joback Method
cpg	1023.40	J/mol×K	1017.37	Joback Method
cpg	1035.94	J/mol×K	1052.24	Joback Method
cpg	1047.50	J/mol×K	1087.10	Joback Method
cpg	1058.12	J/mol×K	1121.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299838&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