4-Cyanobenzoic acid, heptadecyl ester

Inchi: InChI=1S/C25H39NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-28-25(27)24-19-17-
InchiKey: RWCIOCJHQNQQIT-UHFFFAOYSA-N
Formula: C25H39NO2
SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 385.58

Physical Properties

Property code	Value	Unit	Source
gf	161.66	kJ/mol	Joback Method
hf	-414.19	kJ/mol	Joback Method
hfus	58.45	kJ/mol	Joback Method
hvap	93.82	kJ/mol	Joback Method
log10ws	-8.76		Crippen Method
logp	7.586		Crippen Method
mcvol	348.170	ml/mol	McGowan Method
pc	928.94	kPa	Joback Method
rinpol	2750.40		NIST Webbook
tb	981.43	K	Joback Method
tc	1201.55	K	Joback Method
tf	547.60	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.92	J/mol×K	981.43	Joback Method
cpg	1179.62	J/mol×K	1018.12	Joback Method
cpg	1195.04	J/mol×K	1054.80	Joback Method
cpg	1209.23	J/mol×K	1091.49	Joback Method
cpg	1222.27	J/mol×K	1128.17	Joback Method
cpg	1234.21	J/mol×K	1164.86	Joback Method
cpg	1245.13	J/mol×K	1201.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292455&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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