4-Cyanobenzoic acid, tridecyl ester

Inchi: InChI=1S/C21H31NO2/c1-2-3-4-5-6-7-8-9-10-11-12-17-24-21(23)20-15-13-19(18-22)14-
InchiKey: DHAAEECFAMJFPO-UHFFFAOYSA-N
Formula: C21H31NO2
SMILES: CCCCCCCCCCCCCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 329.48

Physical Properties

Property code	Value	Unit	Source
gf	127.98	kJ/mol	Joback Method
hf	-331.63	kJ/mol	Joback Method
hfus	48.09	kJ/mol	Joback Method
hvap	84.91	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.026		Crippen Method
mcvol	291.810	ml/mol	McGowan Method
pc	1191.52	kPa	Joback Method
rinpol	2540.00		NIST Webbook
tb	889.91	K	Joback Method
tc	1097.22	K	Joback Method
tf	502.52	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.48	J/mol×K	889.91	Joback Method
cpg	934.98	J/mol×K	924.46	Joback Method
cpg	949.41	J/mol×K	959.01	Joback Method
cpg	962.79	J/mol×K	993.56	Joback Method
cpg	975.18	J/mol×K	1028.12	Joback Method
cpg	986.61	J/mol×K	1062.67	Joback Method
cpg	997.12	J/mol×K	1097.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299837&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