4-Cyanobenzoic acid, dodecyl ester

Inchi: InChI=1S/C20H29NO2/c1-2-3-4-5-6-7-8-9-10-11-16-23-20(22)19-14-12-18(17-21)13-15-
InchiKey: HBZNFSKEIJSFOA-UHFFFAOYSA-N
Formula: C20H29NO2
SMILES: CCCCCCCCCCCCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 315.45

Physical Properties

Property code	Value	Unit	Source
gf	119.56	kJ/mol	Joback Method
hf	-310.99	kJ/mol	Joback Method
hfus	45.50	kJ/mol	Joback Method
hvap	82.69	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.636		Crippen Method
mcvol	277.720	ml/mol	McGowan Method
pc	1274.60	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	867.03	K	Joback Method
tc	1073.27	K	Joback Method
tf	491.25	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.27	J/mol×K	867.03	Joback Method
cpg	875.52	J/mol×K	901.40	Joback Method
cpg	889.72	J/mol×K	935.78	Joback Method
cpg	902.91	J/mol×K	970.15	Joback Method
cpg	915.14	J/mol×K	1004.52	Joback Method
cpg	926.43	J/mol×K	1038.90	Joback Method
cpg	936.83	J/mol×K	1073.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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