4-Cyanobenzoic acid, butyl ester

Inchi: InChI=1S/C12H13NO2/c1-2-3-8-15-12(14)11-6-4-10(9-13)5-7-11/h4-7H,2-3,8H2,1H3
InchiKey: SRGVIBGHRBGAAS-UHFFFAOYSA-N
Formula: C12H13NO2
SMILES: CCCCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 203.24

Physical Properties

Property code	Value	Unit	Source
gf	52.20	kJ/mol	Joback Method
hf	-145.87	kJ/mol	Joback Method
hfus	24.78	kJ/mol	Joback Method
hvap	64.88	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.515		Crippen Method
mcvol	165.000	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	1593.00		NIST Webbook
tb	683.99	K	Joback Method
tc	904.34	K	Joback Method
tf	401.09	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.49	J/mol×K	683.99	Joback Method
cpg	432.73	J/mol×K	720.72	Joback Method
cpg	444.17	J/mol×K	757.44	Joback Method
cpg	454.83	J/mol×K	794.17	Joback Method
cpg	464.71	J/mol×K	830.89	Joback Method
cpg	473.85	J/mol×K	867.62	Joback Method
cpg	482.26	J/mol×K	904.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299829&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