4-Cyanobenzoic acid, heptyl ester

Inchi: InChI=1S/C15H19NO2/c1-2-3-4-5-6-11-18-15(17)14-9-7-13(12-16)8-10-14/h7-10H,2-6,1
InchiKey: QNDZVAFNIKAYET-UHFFFAOYSA-N
Formula: C15H19NO2
SMILES: CCCCCCCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 245.32

Physical Properties

Property code	Value	Unit	Source
gf	77.46	kJ/mol	Joback Method
hf	-207.79	kJ/mol	Joback Method
hfus	32.55	kJ/mol	Joback Method
hvap	71.56	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.685		Crippen Method
mcvol	207.270	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	1862.00		NIST Webbook
rinpol	1862.00		NIST Webbook
tb	752.63	K	Joback Method
tc	963.66	K	Joback Method
tf	434.90	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.27	J/mol×K	752.63	Joback Method
cpg	591.00	J/mol×K	787.80	Joback Method
cpg	603.83	J/mol×K	822.97	Joback Method
cpg	615.79	J/mol×K	858.15	Joback Method
cpg	626.89	J/mol×K	893.32	Joback Method
cpg	637.17	J/mol×K	928.49	Joback Method
cpg	646.65	J/mol×K	963.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299832&Units=SI

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