Ethyl 4-cyanobenzoate

Other names:	Benzoic acid, 4-cyano-, ethyl ester
	4-Cyanobenzoic acid, ethyl ester
Inchi:	InChI=1S/C10H9NO2/c1-2-13-10(12)9-5-3-8(7-11)4-6-9/h3-6H,2H2,1H3
InchiKey:	JLSSWDFCYXSLQX-UHFFFAOYSA-N
Formula:	C10H9NO2
SMILES:	CCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]:	175.18
CAS:	7153-22-2

Physical Properties

Property code	Value	Unit	Source
gf	35.36	kJ/mol	Joback Method
hf	-104.59	kJ/mol	Joback Method
hfus	19.60	kJ/mol	Joback Method
hvap	60.43	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.735		Crippen Method
mcvol	136.820	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
rinpol	1393.00		NIST Webbook
tb	638.23	K	Joback Method
tc	866.78	K	Joback Method
tf	378.55	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.77	J/mol×K	638.23	Joback Method
cpg	333.55	J/mol×K	676.32	Joback Method
cpg	343.62	J/mol×K	714.41	Joback Method
cpg	352.99	J/mol×K	752.51	Joback Method
cpg	361.68	J/mol×K	790.60	Joback Method
cpg	369.68	J/mol×K	828.69	Joback Method

cpg	377.02	J/mol×K	866.78	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=C7153222&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