

o-Cyanobenzoic acid

Other names:	Benzoic acid, 2-cyano- 2-Cyanobenzoic acid
Inchi:	InChI=1S/C8H5NO2/c9-5-6-3-1-2-4-7(6)8(10)11/h1-4H,(H,10,11)
InchiKey:	DTNSDCJFTHMDAK-UHFFFAOYSA-N
Formula:	C8H5NO2
SMILES:	N#Cc1ccccc1C(=O)O
Mol. weight [g/mol]:	147.13
CAS:	3839-22-3

Physical Properties

Property code	Value	Unit	Source
gf	-13.30	kJ/mol	Joback Method
hf	-83.32	kJ/mol	Joback Method
hfus	17.32	kJ/mol	Joback Method
hsub	114.60 ± 1.30	kJ/mol	NIST Webbook
hvap	70.24	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.256		Crippen Method
mcvol	108.640	ml/mol	McGowan Method
pc	4216.56	kPa	Joback Method
tb	662.23	K	Joback Method
tc	883.54	K	Joback Method
tf	394.60	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.34	J/mol×K	662.23	Joback Method
cpg	254.39	J/mol×K	699.12	Joback Method
cpg	260.92	J/mol×K	736.00	Joback Method
cpg	266.96	J/mol×K	772.89	Joback Method
cpg	272.52	J/mol×K	809.77	Joback Method
cpg	277.64	J/mol×K	846.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3839223&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

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
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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