«beta»-Cyanopropiophenone

Inchi: InChI=1S/C10H9NO/c11-8-4-7-10(12)9-5-2-1-3-6-9/h1-3,5-6H,4,7H2
InchiKey: OSPRTYTUQJCKFF-UHFFFAOYSA-N
Formula: C10H9NO
SMILES: N#CCCC(=O)c1ccccc1
Mol. weight [g/mol]: 159.18
CAS: 5343-98-6

Physical Properties

Property code	Value	Unit	Source
chs	-5149.96 ± 0.46	kJ/mol	NIST Webbook
gf	149.99	kJ/mol	Joback Method
hf	30.00 ± 0.46	kJ/mol	NIST Webbook
hfs	-71.46 ± 0.46	kJ/mol	NIST Webbook
hfus	18.80	kJ/mol	Joback Method
hsub	102.00 ± 4.20	kJ/mol	NIST Webbook
hvap	57.35	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.173		Crippen Method
mcvol	130.950	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
tb	610.83	K	Joback Method
tc	841.68	K	Joback Method
tf	343.80	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.58	J/mol×K	803.21	Joback Method
cpg	301.43	J/mol×K	610.83	Joback Method
cpg	312.59	J/mol×K	649.31	Joback Method
cpg	322.94	J/mol×K	687.78	Joback Method
cpg	332.53	J/mol×K	726.26	Joback Method
cpg	341.40	J/mol×K	764.73	Joback Method

cpg	357.11	J/mol×K	841.68	Joback Method
hsubt	108.50	kJ/mol	325.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5343986&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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