5-Methylisophthalonitrile

Inchi: InChI=1S/C9H6N2/c1-7-2-8(5-10)4-9(3-7)6-11/h2-4H,1H3
InchiKey: LYSGVAGOLJKEGK-UHFFFAOYSA-N
Formula: C9H6N2
SMILES: Cc1cc(C#N)cc(C#N)c1
Mol. weight [g/mol]: 142.16
CAS: 39718-07-5

Physical Properties

Property code	Value	Unit	Source
gf	384.41	kJ/mol	Joback Method
hf	314.26	kJ/mol	Joback Method
hfus	15.34	kJ/mol	Joback Method
hvap	60.18	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.738		Crippen Method
mcvol	116.670	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
tb	646.12	K	Joback Method
tc	890.24	K	Joback Method
tf	372.63	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.47	J/mol×K	646.12	Joback Method
cpg	264.93	J/mol×K	686.81	Joback Method
cpg	272.81	J/mol×K	727.49	Joback Method
cpg	280.11	J/mol×K	768.18	Joback Method
cpg	286.86	J/mol×K	808.87	Joback Method
cpg	293.09	J/mol×K	849.55	Joback Method
cpg	298.83	J/mol×K	890.24	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=C39718075&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume