2,5-Dimethylbenzonitrile

Other names: Benzonitrile, 2,5-dimethyl-
Inchi: InChI=1S/C9H9N/c1-7-3-4-8(2)9(5-7)6-10/h3-5H,1-2H3
InchiKey: OZOQTENKIVKILK-UHFFFAOYSA-N
Formula: C9H9N
SMILES: Cc1ccc(C)c(C#N)c1
Mol. weight [g/mol]: 131.17
CAS: 13730-09-1

Physical Properties

Property code	Value	Unit	Source
gf	251.23	kJ/mol	Joback Method
hf	149.38	kJ/mol	Joback Method
hfus	13.83	kJ/mol	Joback Method
hvap	49.71	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.175		Crippen Method
mcvol	115.290	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	544.04	K	Joback Method
tc	773.77	K	Joback Method
tf	307.64	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.78	J/mol×K	544.04	Joback Method
cpg	253.66	J/mol×K	582.33	Joback Method
cpg	263.89	J/mol×K	620.62	Joback Method
cpg	273.51	J/mol×K	658.91	Joback Method
cpg	282.54	J/mol×K	697.19	Joback Method
cpg	290.99	J/mol×K	735.48	Joback Method
cpg	298.89	J/mol×K	773.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	497.70	K	97.30	NIST Webbook

Sources

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=C13730091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume