2,4-DIMETHYLBENZONITRILE

Other names: 2,6-Dimethylbenzonitrile
Benzonitrile, 2,4-dimethyl-
Inchi: InChI=1S/C9H9N/c1-7-3-4-9(6-10)8(2)5-7/h3-5H,1-2H3
InchiKey: QLZDTHTXOUOSCV-UHFFFAOYSA-N
Formula: C9H9N
SMILES: Cc1ccc(C#N)c(C)c1
Mol. weight [g/mol]: 131.18

Physical Properties

Property code	Value	Unit	Source
af	0.4320		Cheméo Relay (1.0)
gf	251.23	kJ/mol	Joback Method
hf	148.27	kJ/mol	Cheméo Relay (1.0)
hfus	13.83	kJ/mol	Joback Method
hvap	60.21	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
log10ws	-2.73		Cheméo Relay (1.0)
logp	2.175		Crippen Method
mcvol	115.290	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	506.03	K	Cheméo Relay (1.0)
tc	738.41	K	Cheméo Relay (1.0)
tf	309.39	K	Cheméo Relay (1.0)
vc	0.423	m3/kmol	Cheméo Relay (1.0)

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

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21789366&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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