

2,6-Dimethylbenzonitrile

Other names:	Benzonitrile, 2,6-dimethyl-
Inchi:	InChI=1S/C9H9N/c1-7-4-3-5-8(2)9(7)6-10/h3-5H,1-2H3
InchiKey:	QSACPWSIIRFHHR-UHFFFAOYSA-N
Formula:	C9H9N
SMILES:	Cc1cccc(C)c1C#N
Mol. weight [g/mol]:	131.17
CAS:	6575-13-9

Physical Properties

Property code	Value	Unit	Source
chs	-4890.10 ± 1.00	kJ/mol	NIST Webbook
gf	251.23	kJ/mol	Joback Method
hf	146.20 ± 3.20	kJ/mol	NIST Webbook
hfs	62.30 ± 1.50	kJ/mol	NIST Webbook
hfus	13.83	kJ/mol	Joback Method
hsub	83.90 ± 2.80	kJ/mol	NIST Webbook
hsub	83.90	kJ/mol	NIST Webbook
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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.60960e+01
Coeff. B	-4.79956e+03
Coeff. C	-8.74780e+01
Temperature range (K), min.	391.09
Temperature range (K), max.	532.52

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C6575139&Units=SI

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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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