

2,5-Dimethylbenzyl cyanide

Other names:	2,5-Xylylacetonitrile 2,5-Dimethylphenylacetonitrile Benzeneacetonitrile, 2,5-dimethyl- Acetonitrile, (2,5-xylyl)-
Inchi:	InChI=1S/C10H11N/c1-8-3-4-9(2)10(7-8)5-6-11/h3-4,7H,5H2,1-2H3
InchiKey:	HCELRQTHSKCQL-UHFFFAOYSA-N
Formula:	C10H11N
SMILES:	<chem>Cc1ccc(C)c(CC#N)c1</chem>
Mol. weight [g/mol]:	145.20
CAS:	16213-85-7

Physical Properties

Property code	Value	Unit	Source
chl	-5563.00	kJ/mol	NIST Webbook
gf	259.65	kJ/mol	Joback Method
hf	128.74	kJ/mol	Joback Method
hfl	46.00	kJ/mol	NIST Webbook
hfus	16.43	kJ/mol	Joback Method
hvap	51.93	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.370		Crippen Method
mvol	129.380	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	566.92	K	Joback Method
tc	792.35	K	Joback Method
tf	301.00 ± 3.00	K	NIST Webbook
vc	0.513	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.99	J/mol×K	566.92	Joback Method
cpg	298.92	J/mol×K	604.49	Joback Method
cpg	310.17	J/mol×K	642.06	Joback Method

cpg	320.73	J/mol×K	679.64	Joback Method
cpg	330.66	J/mol×K	717.21	Joback Method
cpg	339.96	J/mol×K	754.78	Joback Method
cpg	348.66	J/mol×K	792.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16213857&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

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