

Benzeneacetonitrile, 3,5-dimethyl-

Other names:	(3,5-dimethylphenyl)acetonitrile
Inchi:	InChI=1S/C10H11N/c1-8-5-9(2)7-10(6-8)3-4-11/h5-7H,3H2,1-2H3
InchiKey:	LMUKNQSVBFEUKR-UHFFFAOYSA-N
Formula:	C10H11N
SMILES:	<chem>Cc1cc(C)cc(CC#N)c1</chem>
Mol. weight [g/mol]:	145.20
CAS:	39101-54-7

Physical Properties

Property code	Value	Unit	Source
gf	259.65	kJ/mol	Joback Method
hf	128.74	kJ/mol	Joback Method
hfus	16.43	kJ/mol	Joback Method
hvap	51.93	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.370		Crippen Method
mcvol	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	318.91	K	Joback Method
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=C39101547&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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
hvp:	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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