

Benzeneethanamine, dimethyl-

Inchi:	InChI=1S/C10H15N/c1-9(11-2)8-10-6-4-3-5-7-10/h3-7,9,11H,8H2,1-2H3
InchiKey:	MYWUZJCMWCOHBA-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CNC(C)Cc1ccccc1
Mol. weight [g/mol]:	149.23
CAS:	29088-49-1

Physical Properties

Property code	Value	Unit	Source
gf	232.68	kJ/mol	Joback Method
hf	34.99	kJ/mol	Joback Method
hfus	17.27	kJ/mol	Joback Method
hvap	46.18	kJ/mol	Joback Method
ie	7.70	eV	NIST Webbook
log10ws	-2.41		Crippen Method
logp	1.837		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
tb	504.61	K	Joback Method
tc	715.64	K	Joback Method
tf	266.54	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.75	J/mol×K	504.61	Joback Method
cpg	320.38	J/mol×K	539.78	Joback Method
cpg	335.09	J/mol×K	574.95	Joback Method
cpg	348.92	J/mol×K	610.13	Joback Method
cpg	361.90	J/mol×K	645.30	Joback Method
cpg	374.08	J/mol×K	680.47	Joback Method
cpg	385.49	J/mol×K	715.64	Joback Method

Sources

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=C29088491&Units=SI

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
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

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