2,4-Dimethylbenzenemethanamine

Other names: Benzenemethanamine, 2,4-dimethyl-
Benzylamine, 2,4-dimethyl-
2,4-dimethylbenzylamine
Inchi: InChI=1S/C9H13N/c1-7-3-4-9(6-10)8(2)5-7/h3-5H,6,10H2,1-2H3
InchiKey: GBSUVYGVEQDZPG-UHFFFAOYSA-N
Formula: C9H13N
SMILES: Cc1ccc(CN)c(C)c1
Mol. weight [g/mol]: 135.21
CAS: 94-98-4

Physical Properties

Property code	Value	Unit	Source
gf	184.50	kJ/mol	Joback Method
hf	18.29	kJ/mol	Joback Method
hfus	17.53	kJ/mol	Joback Method
hvap	49.87	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	1.762		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	491.70	K	NIST Webbook
tc	736.31	K	Joback Method
tf	325.91	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.48	J/mol×K	514.49	Joback Method
cpg	284.80	J/mol×K	551.46	Joback Method
cpg	297.37	J/mol×K	588.43	Joback Method
cpg	309.24	J/mol×K	625.40	Joback Method
cpg	320.42	J/mol×K	662.37	Joback Method
cpg	330.93	J/mol×K	699.34	Joback Method

cpg	340.81	J/mol×K	736.31	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.20	K	1.30	NIST Webbook

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=C94984&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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