2,4-Dimethylbenzyl amine

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

Physical Properties

Property code	Value	Unit	Source
af	0.4738		Cheméo Relay (1.0)
gf	184.50	kJ/mol	Joback Method
hf	8.11	kJ/mol	Cheméo Relay (1.0)
hfus	17.53	kJ/mol	Joback Method
hvap	60.65	kJ/mol	Cheméo Relay (1.0)
ie	8.02	eV	Cheméo Relay (1.0)
log10ws	-1.76		Cheméo Relay (1.0)
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	709.42	K	Cheméo Relay (1.0)
tf	271.34	K	Cheméo Relay (1.0)
vc	0.440	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C94984&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume