Benzenemethanamine, 3-methyl-

Other names: 3-Methylbenzylamine
Benzylamine, m-methyl-
m-Methylbenzylamine
Inchi: InChI=1S/C8H11N/c1-7-3-2-4-8(5-7)6-9/h2-5H,6,9H2,1H3
InchiKey: RGXUCUWVGKLACF-UHFFFAOYSA-N
Formula: C8H11N
SMILES: Cc1cccc(CN)c1
Mol. weight [g/mol]: 121.18
CAS: 100-81-2

Physical Properties

Property code	Value	Unit	Source
gf	185.71	kJ/mol	Joback Method
hf	50.40	kJ/mol	Joback Method
hfus	15.32	kJ/mol	Joback Method
hvap	46.98	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	1.454		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
tb	476.70	K	NIST Webbook
tc	710.97	K	Joback Method
tf	302.12	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.77	J/mol×K	486.63	Joback Method
cpg	241.38	J/mol×K	524.02	Joback Method
cpg	253.24	J/mol×K	561.41	Joback Method
cpg	264.37	J/mol×K	598.80	Joback Method
cpg	274.81	J/mol×K	636.19	Joback Method
cpg	284.60	J/mol×K	673.58	Joback Method

cpg	293.75	J/mol×K	710.97	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	2.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100812&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
KDB: https://www.cheric.org/files/research/kdb/mol/mol1398.mol

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