

3,3-DIMETHYLBUTYLAMINE

Other names:	1-Butanamine, 3,3-dimethyl-
Inchi:	InChI=1S/C6H15N/c1-6(2,3)4-5-7/h4-5,7H2,1-3H3
InchiKey:	GPWHFPWZAPOYNO-UHFFFAOYSA-N
Formula:	C6H15N
SMILES:	CC(C)(C)CCN
Mol. weight [g/mol]:	101.19

Physical Properties

Property code	Value	Unit	Source
af	0.3722		Cheméo Relay (1.0)
gf	68.93	kJ/mol	Joback Method
hf	-178.63	kJ/mol	Cheméo Relay (1.0)
hfus	9.08	kJ/mol	Joback Method
hvap	39.31	kJ/mol	Cheméo Relay (1.0)
ie	8.81	eV	Cheméo Relay (1.0)
log10ws	-1.19		Cheméo Relay (1.0)
logp	1.381		Crippen Method
mcvol	105.380	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
tb	388.20	K	NIST Webbook
tc	562.17	K	Cheméo Relay (1.0)
tf	244.90	K	Cheméo Relay (1.0)
vc	0.359	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.86	J/mol×K	405.98	Joback Method
cpg	225.70	J/mol×K	437.99	Joback Method
cpg	237.86	J/mol×K	469.99	Joback Method
cpg	249.37	J/mol×K	502.00	Joback Method
cpg	260.26	J/mol×K	534.01	Joback Method
cpg	270.57	J/mol×K	566.02	Joback Method
cpg	280.31	J/mol×K	598.02	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15673004&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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