1-Butanamine, N,N,3-trimethyl

Other names: Dimethylisoamylamine
Inchi: InChI=1S/C7H17N/c1-7(2)5-6-8(3)4/h7H,5-6H2,1-4H3
InchiKey: KOOQJINBDNZUTB-UHFFFAOYSA-N
Formula: C7H17N
SMILES: CC(C)CCN(C)C
Mol. weight [g/mol]: 115.22

Physical Properties

Property code	Value	Unit	Source
gf	116.40	kJ/mol	Joback Method
hf	-125.56	kJ/mol	Joback Method
hfus	13.38	kJ/mol	Joback Method
hvap	32.83	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	1.594		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
rinpol	754.00		NIST Webbook
rinpol	754.00		NIST Webbook
tb	371.56	K	Joback Method
tc	537.88	K	Joback Method
tf	186.12	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.23	J/mol×K	371.56	Joback Method
cpg	234.61	J/mol×K	399.28	Joback Method
cpg	247.47	J/mol×K	427.00	Joback Method
cpg	259.82	J/mol×K	454.72	Joback Method
cpg	271.66	J/mol×K	482.44	Joback Method
cpg	283.03	J/mol×K	510.16	Joback Method
cpg	293.92	J/mol×K	537.88	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=R12850&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume