1-Butanamine, N-(1-methylethyl)-

Other names: Butylisopropylamine
Isopropylbutylamine
N-Isopropylbutylamine
Butylamine, N-isopropyl-
isopropyl-n-butylamine
Inchi: InChI=1S/C7H17N/c1-4-5-6-8-7(2)3/h7-8H,4-6H2,1-3H3
InchiKey: OKRJGUKZYSEUOY-UHFFFAOYSA-N
Formula: C7H17N
SMILES: CCCCNC(C)C
Mol. weight [g/mol]: 115.22
CAS: 39099-23-5

Physical Properties

Property code	Value	Unit	Source
chl	-4980.90 ± 3.00	kJ/mol	NIST Webbook
gf	95.01	kJ/mol	Joback Method
hf	-165.00 ± 3.70	kJ/mol	NIST Webbook
hfl	-203.20 ± 3.10	kJ/mol	NIST Webbook
hfus	15.46	kJ/mol	Joback Method
hvap	42.08	kJ/mol	NIST Webbook
hvap	42.10 ± 0.10	kJ/mol	NIST Webbook
hvap	38.20	kJ/mol	NIST Webbook
hvap	38.20 ± 2.00	kJ/mol	NIST Webbook
log10ws	-2.05		Crippen Method
logp	1.785		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	795.00		NIST Webbook
rinpol	795.00		NIST Webbook
tb	396.60	K	NIST Webbook
tb	397.15 ± 2.00	K	NIST Webbook
tc	563.60	K	NIST Webbook
tf	206.31	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.14	J/mol×K	409.29	Joback Method
cpg	297.97	J/mol×K	553.50	Joback Method
cpg	286.96	J/mol×K	524.66	Joback Method
cpg	275.48	J/mol×K	495.82	Joback Method
cpg	263.53	J/mol×K	466.97	Joback Method
cpg	251.08	J/mol×K	438.13	Joback Method
cpg	308.53	J/mol×K	582.34	Joback Method
hvapt	40.00	kJ/mol	360.00	NIST Webbook
hvapt	37.60 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	38.70 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	39.90 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	40.90 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	34.52	kJ/mol	396.60	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=C39099235&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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