isobutyl-n-butyl-amine

Other names:	Butylisobutyl amine
	N-isobutylbutylamine
	1-Butanamine, N-(2-methylpropyl)-
Inchi:	InChI=1S/C8H19N/c1-4-5-6-9-7-8(2)3/h8-9H,4-7H2,1-3H3
InchiKey:	CCRUHKGZAQXBKC-UHFFFAOYSA-N
Formula:	C8H19N
SMILES:	CCCCNCC(C)C
Mol. weight [g/mol]:	129.24
CAS:	20810-06-4

Physical Properties

Property code	Value	Unit	Source
chl	-5647.70 ± 5.20	kJ/mol	NIST Webbook
gf	103.43	kJ/mol	Joback Method
hf	-175.00 ± 6.30	kJ/mol	NIST Webbook
hfl	-216.00 ± 5.00	kJ/mol	NIST Webbook
hfus	18.05	kJ/mol	Joback Method
hvap	41.00	kJ/mol	NIST Webbook
log10ws	-2.12		Crippen Method
logp	2.032		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	898.00		NIST Webbook
ripol	1014.00		NIST Webbook
ripol	1014.00		NIST Webbook
tb	432.17	K	Joback Method
tc	604.23	K	Joback Method
tf	217.58	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.20	J/mol×K	546.88	Joback Method

cpg	344.10	J/mol×K	575.56	Joback Method
cpg	279.40	J/mol×K	432.17	Joback Method
cpg	293.41	J/mol×K	460.85	Joback Method
cpg	306.87	J/mol×K	489.52	Joback Method
cpg	319.80	J/mol×K	518.20	Joback Method
cpg	355.50	J/mol×K	604.23	Joback Method
hvapt	41.20	kJ/mol	368.00	NIST Webbook
hvapt	41.00 ± 1.00	kJ/mol	313.00	NIST Webbook

Sources

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=C20810064&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume