

N-Isobutyl-sec-butylamine

Other names:	2-Butanamine, N-(2-methylpropyl)- 1-Propanamine, 2-methyl, N-(1-methylpropyl)
Inchi:	InChI=1S/C8H19N/c1-5-8(4)9-6-7(2)3/h7-9H,5-6H2,1-4H3
InchiKey:	DVFVBAPHBZWJFX-UHFFFAOYSA-N
Formula:	C8H19N
SMILES:	CCC(C)NCC(C)C
Mol. weight [g/mol]:	129.24
CAS:	39190-88-0

Physical Properties

Property code	Value	Unit	Source
gf	100.99	kJ/mol	Joback Method
hf	-165.54	kJ/mol	Joback Method
hfus	14.53	kJ/mol	Joback Method
hvap	39.06	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.030		Crippen Method
mvol	133.560	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
rinpol	843.00		NIST Webbook
tb	431.73	K	Joback Method
tc	607.62	K	Joback Method
tf	202.58	K	Joback Method
vc	0.506	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.42	J/mol×K	431.73	Joback Method
cpg	293.82	J/mol×K	461.04	Joback Method
cpg	307.65	J/mol×K	490.36	Joback Method
cpg	320.91	J/mol×K	519.67	Joback Method
cpg	333.62	J/mol×K	548.99	Joback Method
cpg	345.79	J/mol×K	578.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39190880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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

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