2-Butanamine, N-methyl-

Other names:	sec-Butylmethylamine
	Propylamine, N,1-dimethyl-
	N-Methyl-sec-butylamine
	N-Methyl-N-sec-butylamine
	N-Methyl-2-butylamine
	N,1-Dimethylpropylamine
	2-(Methylamino)butane
	N-(sec-Butyl)-N-methylamine
Inchi:	InChI=1S/C5H13N/c1-4-5(2)6-3/h5-6H,4H2,1-3H3
InchiKey:	PYFSCIWXNSXGNS-UHFFFAOYSA-N
Formula:	C5H13N
SMILES:	CCC(C)NC
Mol. weight [g/mol]:	87.16
CAS:	7713-69-1

Physical Properties

Property code	Value	Unit	Source
hf	-90.07	kJ/mol	Cheméo Relay (1.0)
hfus	10.28	kJ/mol	Joback Method
hvap	35.61	kJ/mol	Cheméo Relay (1.0)
ie	8.08	eV	Cheméo Relay (1.0)
log10ws	0.23		Cheméo Relay (1.0)
logp	1.004		Crippen Method
mcvol	91.290	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	652.00		NIST Webbook
rinpol	652.00		NIST Webbook
tb	351.65 ± 2.00	K	NIST Webbook
tc	531.55	K	Cheméo Relay (1.0)
tf	200.47	K	Cheméo Relay (1.0)
vc	0.342	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-4.54900e+00
Coeff. B	5.60960e-01
Coeff. C	-3.00000e-04
Coeff. D	5.83000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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=C7713691&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
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
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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