

1-Butanamine, N-propyl-

Other names:	Butylamine, N-propyl- Butylpropylamine N-Butyl-N-propylamine N-Propyl-1-butylamine N-Propylbutylamine propylbutyl-amine
Inchi:	InChI=1S/C7H17N/c1-3-5-7-8-6-4-2/h8H,3-7H2,1-2H3
InchiKey:	CWYZDPHNAGSFQB-UHFFFAOYSA-N
Formula:	C7H17N
SMILES:	CCCCNCCC
Mol. weight [g/mol]:	115.22
CAS:	20193-21-9

Physical Properties

Property code	Value	Unit	Source
gf	97.45	kJ/mol	Joback Method
hf	-134.34	kJ/mol	Joback Method
hfus	18.98	kJ/mol	Joback Method
hvap	37.61	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.786		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpola	847.00		NIST Webbook
tb	409.73	K	Joback Method
tc	578.95	K	Joback Method
tf	221.31	K	Joback Method
vc	0.463	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.17	J/mol×K	409.73	Joback Method
cpg	250.74	J/mol×K	437.93	Joback Method

cpg	262.84	J/mol×K	466.14	Joback Method
cpg	274.48	J/mol×K	494.34	Joback Method
cpg	285.67	J/mol×K	522.55	Joback Method
cpg	296.42	J/mol×K	550.75	Joback Method
cpg	306.74	J/mol×K	578.95	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54299e+01
Coeff. B	-3.83283e+03
Coeff. C	-5.41990e+01
Temperature range (K), min.	307.32
Temperature range (K), max.	433.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C20193219&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
pvap:	Vapor 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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