

1,3-Butanediamine

Other names:	1,3-Diaminobutane 1-methyltrimethylenediamine
Inchi:	InChI=1S/C4H12N2/c1-4(6)2-3-5/h4H,2-3,5-6H2,1H3
InchiKey:	RGTXVXDNHPWPHH-UHFFFAOYSA-N
Formula:	C4H12N2
SMILES:	CC(N)CCN
Mol. weight [g/mol]:	88.15
CAS:	590-88-5

Physical Properties

Property code	Value	Unit	Source
gf	113.26	kJ/mol	Joback Method
hf	-63.59	kJ/mol	Joback Method
hfus	12.99	kJ/mol	Joback Method
hvap	45.39	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	-0.318		Crippen Method
mvol	87.180	ml/mol	McGowan Method
pc	4565.38	kPa	Joback Method
tb	435.54	K	Joback Method
tc	637.55	K	Joback Method
tf	286.36	K	Joback Method
vc	0.311	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.16	J/mol×K	435.54	Joback Method
cpg	195.00	J/mol×K	469.21	Joback Method
cpg	204.38	J/mol×K	502.88	Joback Method
cpg	213.32	J/mol×K	536.55	Joback Method
cpg	221.83	J/mol×K	570.22	Joback Method
cpg	229.91	J/mol×K	603.88	Joback Method
cpg	237.60	J/mol×K	637.55	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.09137e+01
Coeff. B	-5.35549e+03
Coeff. C	-5.76740e+01
Temperature range (K), min.	317.32
Temperature range (K), max.	400.93

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/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=C590885&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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