

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
hf	-86.94	kJ/mol	Cheméo Relay (1.0)
hfus	12.99	kJ/mol	Joback Method
hvap	43.38	kJ/mol	Cheméo Relay (1.0)
ie	8.78	eV	Cheméo Relay (1.0)
logp	-0.318		Crippen Method
mcvol	87.180	ml/mol	McGowan Method
pc	4565.38	kPa	Joback Method
tb	410.05	K	Cheméo Relay (1.0)
tc	599.10	K	Cheméo Relay (1.0)
tf	228.47	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C590885&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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

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