Di(3-Methylbutyl)amine

Other names: 1-Butanamine, 3-methyl-N-(3-methylbutyl)-
Diisoamylamine
Diisopentylamine
Inchi: InChI=1S/C10H23N/c1-9(2)5-7-11-8-6-10(3)4/h9-11H,5-8H2,1-4H3
InchiKey: SPVVMXMTSODFPU-UHFFFAOYSA-N
Formula: C10H23N
SMILES: CC(C)CCNCCC(C)C
Mol. weight [g/mol]: 157.30
CAS: 544-00-3

Physical Properties

Property code	Value	Unit	Source
chl	-6974.30	kJ/mol	NIST Webbook
gf	117.83	kJ/mol	Joback Method
hf	-206.82	kJ/mol	Joback Method
hfl	-248.00	kJ/mol	NIST Webbook
hfus	19.71	kJ/mol	Joback Method
hvap	43.51	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.668		Crippen Method
mcvol	161.740	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1046.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1061.00		NIST Webbook
tb	461.20	K	NIST Webbook
tc	650.76	K	Joback Method
tf	225.12	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.34	J/mol×K	477.49	Joback Method

cpg	384.54	J/mol×K	506.37	Joback Method
cpg	400.08	J/mol×K	535.25	Joback Method
cpg	414.98	J/mol×K	564.12	Joback Method
cpg	429.25	J/mol×K	593.00	Joback Method
cpg	442.91	J/mol×K	621.88	Joback Method
cpg	455.97	J/mol×K	650.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56757e+01
Coeff. B	-4.33283e+03
Coeff. C	-6.93500e+01
Temperature range (K), min.	350.92
Temperature range (K), max.	487.41

Sources

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=C544003&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase 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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