

2-Pentamine, 2,4,4-trimethyl-

Other names:	1,1,3,3-Tetramethylbutanamine 1,1,3,3-Tetramethylbutylamine 2,4,4-Trimethyl-2-Pentylamine Butylamine, 1,1,3,3-tetramethyl- Butylamine, bis(1,3-dimethyl)- NSC 33852 t-Octylamine tert-Octylamine
Inchi:	InChI=1S/C8H19N/c1-7(2,3)6-8(4,5)9/h6,9H2,1-5H3
InchiKey:	QJIUJYANDSEKG-UHFFFAOYSA-N
Formula:	C8H19N
SMILES:	CC(C)(C)CC(C)(C)N
Mol. weight [g/mol]:	129.24
CAS:	107-45-9

Physical Properties

Property code	Value	Unit	Source
gf	88.61	kJ/mol	Joback Method
hf	-192.16	kJ/mol	Joback Method
hfus	6.84	kJ/mol	Joback Method
hvap	41.45	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.160		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	873.60		NIST Webbook
rinpol	885.00		NIST Webbook
tb	413.15 ± 2.00	K	NIST Webbook
tb	413.20	K	NIST Webbook
tc	649.55	K	Joback Method
tf	268.02	K	Joback Method
vc	0.490	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.32	J/molxK	448.51	Joback Method
cpg	313.73	J/molxK	482.02	Joback Method
cpg	329.12	J/molxK	515.52	Joback Method
cpg	343.54	J/molxK	549.03	Joback Method
cpg	357.06	J/molxK	582.53	Joback Method
cpg	369.71	J/molxK	616.04	Joback Method
cpg	381.57	J/molxK	649.55	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56522e+01
Coeff. B	-3.94125e+03
Coeff. C	-5.60060e+01
Temperature range (K), min.	312.52
Temperature range (K), max.	437.14

Sources

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=C107459&Units=SI
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

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
hvac:	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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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