

Octodrine

Other names:	1,5-Dimethylhexanamine 1,5-Dimethylhexylamine 2-Amino-6-Methylheptane 2-Heptanamine, 6-methyl- 2-Heptylamine, 6-methyl- 2-Isooctylamine 2-Methyl-6-aminoheptane 2-Metil-6-amino-eptano 6-Amino-2-methylheptane 6-Methyl-2-heptylamine Amidrine Hexylamine, 1,5-dimethyl- Isoctaminum Octodrin SK&F-51 SKF 51 Vaporpac «alpha»,«epsilon»-Dimethylhexylamine Â«alphaÂ»,Â«epsilonÂ»-Dimethylhexylamine
Inchi:	InChI=1S/C8H19N/c1-7(2)5-4-6-8(3)9/h7-8H,4-6,9H2,1-3H3
InchiKey:	QNIVIMYXGGFTAK-UHFFFAOYSA-N
Formula:	C8H19N
SMILES:	CC(C)CCCC(C)N
Mol. weight [g/mol]:	129.24
CAS:	543-82-8

Physical Properties

Property code	Value	Unit	Source
gf	78.05	kJ/mol	Joback Method
hf	-185.22	kJ/mol	Joback Method
hfus	14.63	kJ/mol	Joback Method
hvap	43.27	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.160		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinpol	923.00		NIST Webbook

ripol	1132.00		NIST Webbook
tb	428.20	K	NIST Webbook
tc	639.32	K	Joback Method
tf	233.18	K	Joback Method
vc	0.500	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.77	J/mol×K	454.09	Joback Method
cpg	307.18	J/mol×K	484.96	Joback Method
cpg	320.97	J/mol×K	515.83	Joback Method
cpg	334.15	J/mol×K	546.71	Joback Method
cpg	346.76	J/mol×K	577.58	Joback Method
cpg	358.79	J/mol×K	608.45	Joback Method
cpg	370.27	J/mol×K	639.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56600e+01
Coeff. B	-4.06362e+03
Coeff. C	-6.01760e+01
Temperature range (K), min.	298.15
Temperature range (K), max.	452.85

Sources

The Yaws Handbook of Vapor
Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<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>

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/32-478-6/Octodrine.pdf>

Generated by Cheméo on 2025-12-05 09:32:51.46460757 +0000 UTC m=+4675368.994648224.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.