

octadec-9-en-1-amine

Inchi:	InChI=1S/C18H37N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h9-10H,2-8,11-1
InchiKey:	QGLWBTPVKHMHVHM-UHFFFAOYSA-N
Formula:	C18H37N
SMILES:	CCCCCCCCC=CCCCCCCCCN
Mol. weight [g/mol]:	267.50
CAS:	112-90-3

Physical Properties

Property code	Value	Unit	Source
af	0.8196		Cheméo Relay (1.0)
gf	247.35	kJ/mol	Joback Method
hf	-343.30	kJ/mol	Cheméo Relay (1.0)
hfus	47.77	kJ/mol	Joback Method
hvap	100.77	kJ/mol	Cheméo Relay (1.0)
ie	8.39	eV	Cheméo Relay (1.0)
log10ws	-6.67		Cheméo Relay (1.0)
logp	5.983		Crippen Method
mcvol	270.160	ml/mol	McGowan Method
pc	1242.46	kPa	Joback Method
tb	603.56	K	Cheméo Relay (1.0)
tc	769.38	K	Cheméo Relay (1.0)
tf	298.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	1.031	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-2.11650e+01
Coeff. B	1.79572e+00

Coeff. C	-1.08260e-03
Coeff. D	2.61400e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

https://en.wikipedia.org/wiki/Joback_method

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):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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