1-Octanamine, N,N-diethyl-

Other names: diethyloctylamine
Inchi: InChI=1S/C12H27N/c1-4-7-8-9-10-11-12-13(5-2)6-3/h4-12H2,1-3H3
InchiKey: BVUGARXRRGZONH-UHFFFAOYSA-N
Formula: C12H27N
SMILES: CCCCCCCCN(CC)CC
Mol. weight [g/mol]: 185.35
CAS: 4088-37-3

Physical Properties

Property code	Value	Unit	Source
gf	160.94	kJ/mol	Joback Method
hf	-223.48	kJ/mol	Joback Method
hfus	29.86	kJ/mol	Joback Method
hvap	44.35	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.689		Crippen Method
mcvol	189.920	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	1244.00		NIST Webbook
rinpol	1244.00		NIST Webbook
tb	486.40	K	Joback Method
tc	646.21	K	Joback Method
tf	257.47	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.92	J/mol×K	486.40	Joback Method
cpg	459.32	J/mol×K	513.04	Joback Method
cpg	476.04	J/mol×K	539.67	Joback Method
cpg	492.09	J/mol×K	566.31	Joback Method
cpg	507.50	J/mol×K	592.94	Joback Method
cpg	522.28	J/mol×K	619.58	Joback Method

cpg	536.45	J/mol×K	646.21	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50905e+01
Coeff. B	-4.36123e+03
Coeff. C	-7.63000e+01
Temperature range (K), min.	370.92
Temperature range (K), max.	522.28

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=C4088373&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/ci990307l
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
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