1-Hexadecanamine, N-ethyl

Inchi: InChI=1S/C18H39N/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-4-2/h19H,3-18H2,1-2
InchiKey: WMQYCVWUHCDVNS-UHFFFAOYSA-N
Formula: C18H39N
SMILES: CCCCCCCCCCCCCCCCNCC
Mol. weight [g/mol]: 269.51

Physical Properties

Property code	Value	Unit	Source
gf	190.07	kJ/mol	Joback Method
hf	-361.38	kJ/mol	Joback Method
hfus	47.48	kJ/mol	Joback Method
hvap	62.10	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	6.077		Crippen Method
mcvol	274.460	ml/mol	McGowan Method
pc	1162.45	kPa	Joback Method
rinpol	1953.00		NIST Webbook
tb	661.41	K	Joback Method
tc	824.88	K	Joback Method
tf	345.28	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.83	J/mol×K	661.41	Joback Method
cpg	811.62	J/mol×K	688.66	Joback Method
cpg	830.58	J/mol×K	715.90	Joback Method
cpg	848.73	J/mol×K	743.15	Joback Method
cpg	866.09	J/mol×K	770.39	Joback Method
cpg	882.69	J/mol×K	797.64	Joback Method
cpg	898.57	J/mol×K	824.88	Joback Method

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=R540019&Units=SI

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
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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