

Hexadecanamide, N-(2-hydroxyethyl)-

Inchi: InChI=1S/C18H37NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18(21)19-16-17-20/h20H,2
InchiKey: HXYVTAGFYLMHSO-UHFFFAOYSA-N
Formula: C18H37NO2
SMILES: CCCCCCCCCCCCCCCC(=O)NCCO
Mol. weight [g/mol]: 299.50

Physical Properties

Property code	Value	Unit	Source
af	1.1332		Cheméo Relay (1.0)
gf	-75.67	kJ/mol	Joback Method
hf	-729.54	kJ/mol	Cheméo Relay (1.0)
hfus	53.16	kJ/mol	Joback Method
hvap	123.32	kJ/mol	Cheméo Relay (1.0)
ie	9.62	eV	Cheméo Relay (1.0)
log10ws	-4.93		Cheméo Relay (1.0)
logp	4.576		Crippen Method
mcvol	281.900	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
tb	627.56	K	Cheméo Relay (1.0)
tc	838.18	K	Cheméo Relay (1.0)
tf	357.70	K	Cheméo Relay (1.0)
vc	1.073	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.75	J/mol×K	807.46	Joback Method
cpg	915.72	J/mol×K	837.76	Joback Method
cpg	931.81	J/mol×K	868.07	Joback Method
cpg	947.06	J/mol×K	898.37	Joback Method
cpg	961.51	J/mol×K	928.67	Joback Method
cpg	975.19	J/mol×K	958.98	Joback Method
cpg	988.13	J/mol×K	989.28	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C544310
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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