HEXANOIC ACID, (2-HEXANOYLAMINOETHYL)-AMIDE

Other names: N-[2-(1-oxohexylamino)ethyl]hexanamide
Inchi: InChI=1S/C14H28N2O2/c1-3-5-7-9-13(17)15-11-12-16-14(18)10-8-6-4-2/h3-12H2,1-2H3
InchiKey: JUFADMDNFLYBPC-UHFFFAOYSA-N
Formula: C14H28N2O2
SMILES: CCCCCC(=O)NCCNC(=O)CCCCC
Mol. weight [g/mol]: 256.39

Physical Properties

Property code	Value	Unit	Source
af	0.8556		Cheméo Relay (1.0)
gf	-12.06	kJ/mol	Joback Method
hf	-619.06	kJ/mol	Cheméo Relay (1.0)
hfus	45.41	kJ/mol	Joback Method
hvap	95.01	kJ/mol	Cheméo Relay (1.0)
ie	9.27	eV	Cheméo Relay (1.0)
log10ws	-3.11		Aqueous Solubility Prediction Method
logp	2.379		Crippen Method
mcvol	231.220	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
tb	581.78	K	Cheméo Relay (1.0)
tc	802.44	K	Cheméo Relay (1.0)
tf	351.03	K	Cheméo Relay (1.0)
vc	0.866	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.94	J/mol×K	727.80	Joback Method
cpg	697.34	J/mol×K	758.16	Joback Method
cpg	711.93	J/mol×K	788.52	Joback Method
cpg	725.74	J/mol×K	818.87	Joback Method
cpg	738.80	J/mol×K	849.23	Joback Method
cpg	751.14	J/mol×K	879.59	Joback Method

cpg	762.77	J/mol×K	909.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50905129&Units=SI
Joback Method:	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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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