Hexanamide, N-hexyl

Inchi: InChI=1S/C12H25NO/c1-3-5-7-9-11-13-12(14)10-8-6-4-2/h3-11H2,1-2H3,(H,13,14)
InchiKey: CKQIYVUVMRSSLI-UHFFFAOYSA-N
Formula: C12H25NO
SMILES: CCCCCCNC(=O)CCCCC
Mol. weight [g/mol]: 199.33

Physical Properties

Property code	Value	Unit	Source
gf	10.63	kJ/mol	Joback Method
hf	-350.12	kJ/mol	Joback Method
hfus	33.53	kJ/mol	Joback Method
hvap	55.49	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.263		Crippen Method
mcvol	191.490	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	1642.00		NIST Webbook
tb	578.00	K	Joback Method
tc	750.80	K	Joback Method
tf	327.59	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.69	J/mol×K	578.00	Joback Method
cpg	508.58	J/mol×K	606.80	Joback Method
cpg	523.77	J/mol×K	635.60	Joback Method
cpg	538.29	J/mol×K	664.40	Joback Method
cpg	552.15	J/mol×K	693.20	Joback Method
cpg	565.39	J/mol×K	722.00	Joback Method
cpg	578.00	J/mol×K	750.80	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=R50707&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