Propanamide, 2-methyl-N-ethyl-N-hexyl-

Inchi: InChI=1S/C12H25NO/c1-5-7-8-9-10-13(6-2)12(14)11(3)4/h11H,5-10H2,1-4H3
InchiKey: HERFYXCXIPFJLM-UHFFFAOYSA-N
Formula: C12H25NO
SMILES: CCCCCCN(CC)C(=O)C(C)C
Mol. weight [g/mol]: 199.33

Physical Properties

Property code	Value	Unit	Source
gf	29.58	kJ/mol	Joback Method
hf	-341.34	kJ/mol	Joback Method
hfus	27.93	kJ/mol	Joback Method
hvap	50.71	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	3.071		Crippen Method
mcvol	191.490	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	1831.00		NIST Webbook
rinpol	1831.00		NIST Webbook
tb	539.83	K	Joback Method
tc	711.68	K	Joback Method
tf	292.40	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.91	J/mol×K	539.83	Joback Method
cpg	489.75	J/mol×K	568.47	Joback Method
cpg	505.84	J/mol×K	597.11	Joback Method
cpg	521.21	J/mol×K	625.75	Joback Method
cpg	535.88	J/mol×K	654.39	Joback Method
cpg	549.87	J/mol×K	683.04	Joback Method
cpg	563.21	J/mol×K	711.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415345&Units=SI
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

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