Butanamide, N-hexyl-3-methyl

Inchi: InChI=1S/C11H23NO/c1-4-5-6-7-8-12-11(13)9-10(2)3/h10H,4-9H2,1-3H3,(H,12,13)
InchiKey: PZJQRNSSYCNVMU-UHFFFAOYSA-N
Formula: C11H23NO
SMILES: CCCCCCN=C(O)CC(C)C
Mol. weight [g/mol]: 185.31

Physical Properties

Property code	Value	Unit	Source
hf	-355.45	kJ/mol	Joback Method
hvap	59.77	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.569		Crippen Method
mcvol	177.400	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	1469.00		NIST Webbook
tb	619.38	K	Joback Method
tc	796.97	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R50494&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

hf: Enthalpy of formation 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

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