Isobutyramide, N-(hept-2-yl)-

Inchi: InChI=1S/C11H23NO/c1-5-6-7-8-10(4)12-11(13)9(2)3/h9-10H,5-8H2,1-4H3,(H,12,13)
InchiKey: FGPZKZODRDQDKQ-UHFFFAOYSA-N
Formula: C11H23NO
SMILES: CCCCCC(C)N=C(O)C(C)C
Mol. weight [g/mol]: 185.31

Physical Properties

Property code	Value	Unit	Source
hf	-360.73	kJ/mol	Joback Method
hvap	59.38	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.568		Crippen Method
mcvol	177.400	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1379.00		NIST Webbook
rinpol	1379.00		NIST Webbook
tb	618.94	K	Joback Method
tc	799.45	K	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=U407090&Units=SI

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