

Hexanamide, N-isobutyl

Inchi: InChI=1S/C10H21NO/c1-4-5-6-7-10(12)11-8-9(2)3/h9H,4-8H2,1-3H3,(H,11,12)
InchiKey: GALBASZQDFWTEP-UHFFFAOYSA-N
Formula: C10H21NO
SMILES: CCCCCC(O)=NCC(C)C
Mol. weight [g/mol]: 171.28

Physical Properties

Property code	Value	Unit	Source
hf	-334.81	kJ/mol	Joback Method
hvap	57.54	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	3.179		Crippen Method
mcvol	163.310	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1372.00		NIST Webbook
rinpol	1372.00		NIST Webbook
tb	596.50	K	Joback Method
tc	775.40	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R50711&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
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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