Hexanamide, N-butyl

Inchi: InChI=1S/C10H21NO/c1-3-5-7-8-10(12)11-9-6-4-2/h3-9H2,1-2H3,(H,11,12)
InchiKey: ZEBBGLVPWGCPJN-UHFFFAOYSA-N
Formula: C10H21NO
SMILES: CCCCCC(O)=NCCCC
Mol. weight [g/mol]: 171.28

Physical Properties

Property code	Value	Unit	Source
hf	-329.53	kJ/mol	Joback Method
hvap	57.93	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	3.323		Crippen Method
mcvol	163.310	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1425.00		NIST Webbook
tb	596.94	K	Joback Method
tc	772.83	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=R50672&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