

Butyramide, 4-hydroxy-n-(2-hydroxyethyl)-

Inchi:	InChI=1S/C6H13NO3/c8-4-1-2-6(10)7-3-5-9/h8-9H,1-5H2,(H,7,10)
InchiKey:	MFHPPMMWHSMDSI-UHFFFAOYSA-N
Formula:	C6H13NO3
SMILES:	OCCCC(O)=NCCO
Mol. weight [g/mol]:	147.17
CAS:	66857-17-8

Physical Properties

Property code	Value	Unit	Source
hf	-551.43	kJ/mol	Joback Method
hvap	82.38	kJ/mol	Joback Method
log10ws	0.16		Crippen Method
logp	-0.292		Crippen Method
mcvol	118.690	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
tb	689.78	K	Joback Method
tc	861.91	K	Joback Method

Sources

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=C66857178&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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