Isobutyramide, N-hexadecyl-

Inchi: InChI=1S/C20H41NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-20(22)19(2)3/h19H
InchiKey: ZNXFIGSGUDJXIF-UHFFFAOYSA-N
Formula: C20H41NO
SMILES: CCCCCCCCCCCCCCCCN=C(O)C(C)C
Mol. weight [g/mol]: 311.55

Physical Properties

Property code	Value	Unit	Source
hf	-541.21	kJ/mol	Joback Method
hvap	79.80	kJ/mol	Joback Method
log10ws	-6.94		Crippen Method
logp	7.080		Crippen Method
mcvol	304.210	ml/mol	McGowan Method
pc	1015.53	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
tb	825.30	K	Joback Method
tc	1011.44	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=U407100&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature