Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-

Other names: 3-Isobutylhexahydropyrrolo[1,2-a]pyrazine-1,4-dione
Cyclo(leucyloprolyl)
Cyclo-Leu-Pro-diketopiperazine

Inchi: InChI=1S/C11H18N2O2/c1-7(2)6-8-11(15)13-5-3-4-9(13)10(14)12-8/h7-9H,3-6H2,1-2H3,

InchiKey: SZJNCZMRZAUNQT-UHFFFAOYSA-N

Formula: C11H18N2O2

SMILES: CC(C)CC1NC(=O)C2CCCN2C1=O

Mol. weight [g/mol]: 210.27

CAS: 5654-86-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.51		Crippen Method
logp	0.522		Crippen Method
mcvol	167.230	ml/mol	McGowan Method
rinpol	1908.00		NIST Webbook
rinpol	1908.00		NIST Webbook
ripol	2870.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5654864&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices