C6306543

Inchi: InChI=1S/C13H13NO4/c1-7(2)10(13(17)18)14-11(15)8-5-3-4-6-9(8)12(14)16/h3-7,10H,1-
InchiKey: UUIPGCXIZVZSEC-JTQLQIEISA-N
Formula: C13H13NO4
SMILES: CC(C)[C@H](C(=O)O)N1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 247.25

Physical Properties

Property code	Value	Unit	Source
hf	-615.43	kJ/mol	Cheméo Relay (1.0)
ie	9.16	eV	Cheméo Relay (1.0)
logp	1.392		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
tb	608.30	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6306543&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

hf: Enthalpy of formation at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature