

C29588838

Inchi: InChI=1S/C11H9NO4/c1-6(11(15)16)12-9(13)7-4-2-3-5-8(7)10(12)14/h2-6H,1H3,(H,15,16)
InchiKey: OZWUITKBAWTEAQ-LURJTMIESA-N
Formula: C11H9NO4
SMILES: C[C@H](C(=O)O)N1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 219.20

Physical Properties

Property code	Value	Unit	Source
hf	-589.37	kJ/mol	Cheméo Relay (1.0)
ie	9.26	eV	Cheméo Relay (1.0)
log10ws	-1.91		Cheméo Relay (1.0)
logp	0.756		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
tb	605.80	K	Cheméo Relay (1.0)
tf	491.28	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C29588838&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

Legend

hf: Enthalpy of formation at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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