PHTHALYL-beta-ALANINE

Other names:	Phthalyl-«beta»-alanine
	3-Phthalimidopropionic acid
	1,3-dihydro-1,3-dioxo-2H-isoindole-2-propionic acid
Inchi:	InChI=1S/C11H9NO4/c13-9(14)5-6-12-10(15)7-3-1-2-4-8(7)11(12)16/h1-4H,5-6H2,(H,13
InchiKey:	DXXHRZUOTPMGEH-UHFFFAOYSA-N
Formula:	C11H9NO4
SMILES:	O=C(O)CCN1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]:	219.20

Physical Properties

Property code	Value	Unit	Source
hf	-575.36	kJ/mol	Cheméo Relay (1.0)
ie	9.41	eV	Cheméo Relay (1.0)
log10ws	-2.03		Cheméo Relay (1.0)
logp	0.757		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	3257.50	kPa	Cheméo Relay (1.0, beta)
tb	621.15	K	Cheméo Relay (1.0)
tf	440.70	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3339739&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point