Isonipecotic acid, N-butoxycarbonyl-, butyl ester

Inchi: InChI=1S/C15H27NO4/c1-3-5-11-19-14(17)13-7-9-16(10-8-13)15(18)20-12-6-4-2/h13H,3

InchiKey: WKLOYJBELNGJNJ-UHFFFAOYSA-N

Formula: C15H27NO4

SMILES: CCCCOC(=O)C1CCN(C(=O)OCCCC)CC1

Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
af	0.7955		Cheméo Relay (1.0)
hf	-870.68	kJ/mol	Cheméo Relay (1.0)
hvap	87.38	kJ/mol	Cheméo Relay (1.0)
ie	8.97	eV	Cheméo Relay (1.0)
log10ws	-2.53		Cheméo Relay (1.0)
logp	2.978		Crippen Method
mcvol	236.210	ml/mol	McGowan Method
pc	1636.04	kPa	Cheméo Relay (1.0, beta)
rinpol	2085.00		NIST Webbook
tb	609.20	K	Cheméo Relay (1.0)
tc	799.15	K	Cheméo Relay (1.0)
tf	267.10	K	Cheméo Relay (1.0)
vc	0.880	m3/kmol	Cheméo Relay (1.0)

Sources

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U322048&Units=SI

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

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume