Isonipecotic acid, N-butoxycarbonyl-, pentadecyl ester

Inchi: InChI=1S/C26H49NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-23-30-25(28)24-18-20-27(

InchiKey: OJWSGJXQJWWKAL-UHFFFAOYSA-N

Formula: C26H49NO4

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

Mol. weight [g/mol]: 439.68

Physical Properties

Property code	Value	Unit	Source
hvap	126.96	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.27		Cheméo Relay (1.0)
logp	7.269		Crippen Method
mcvol	391.200	ml/mol	McGowan Method
tb	684.72	K	Cheméo Relay (1.0)
tf	305.37	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=U322059&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

hvap: Enthalpy of vaporization at standard conditions

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