Isonipecotic acid, N-benzoyl-, propyl ester

Inchi: InChI=1S/C16H21NO3/c1-2-12-20-16(19)14-8-10-17(11-9-14)15(18)13-6-4-3-5-7-13/h3-
InchiKey: JUEQUMTYGYSLEP-UHFFFAOYSA-N
Formula: C16H21NO3
SMILES: CCCOC(=O)C1CCN(C(=O)c2ccccc2)CC1
Mol. weight [g/mol]: 275.35

Physical Properties

Property code	Value	Unit	Source
af	0.6779		Cheméo Relay (1.0)
ie	8.85	eV	Cheméo Relay (1.0)
log10ws	-2.94		Cheméo Relay (1.0)
logp	2.492		Crippen Method
mcvol	220.670	ml/mol	McGowan Method
pc	1665.49	kPa	Cheméo Relay (1.0, beta)
rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook
tb	643.38	K	Cheméo Relay (1.0)
tc	861.34	K	Cheméo Relay (1.0)
tf	325.62	K	Cheméo Relay (1.0)
vc	0.793	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360971&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):

Legend

af:	Acentric Factor
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

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