

3-Pyridinecarboxylic acid, phenylmethyl ester

Other names:	3-Pyridinecarboxylic acid, phenylmethyl ester Benzyl nicotinate Benzyl pyridine-3-carboxylate Niacin benzyl ester Pyridine-3-carboxylic acid benzyl ester Rubriment Estru benzyłowego kwasu nikotynowego Pycaril Pykaryl Nicotinic acid, phenylmethyl ester
Inchi:	InChI=1S/C13H11NO2/c15-13(12-7-4-8-14-9-12)16-10-11-5-2-1-3-6-11/h1-9H,10H2
InchiKey:	KVYGGMBOZFWZBQ-UHFFFAOYSA-N
Formula:	C13H11NO2
SMILES:	O=C(OCc1ccccc1)c1ccnc1
Mol. weight [g/mol]:	213.24

Physical Properties

Property code	Value	Unit	Source
af	0.5801		Cheméo Relay (1.0)
hf	-88.72	kJ/mol	Cheméo Relay (1.0)
hvap	83.49	kJ/mol	Cheméo Relay (1.0)
ie	9.09	eV	Cheméo Relay (1.0)
log10ws	-2.80		Cheméo Relay (1.0)
logp	2.439		Crippen Method
mcvol	163.930	ml/mol	McGowan Method
pc	3036.33	kPa	Cheméo Relay (1.0, beta)
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	590.74	K	Cheméo Relay (1.0)
tc	868.57	K	Cheméo Relay (1.0)
tf	298.27	K	Cheméo Relay (1.0)

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C94440&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):
Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
h_{vap}:	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

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