

OCTADECYL NICOTINATE

Other names:	Nicotinic acid, octadecyl ester
Inchi:	InChI=1S/C24H41NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-27-24(26)23-19-
InchiKey:	LCMBGJRROPDVAA-UHFFFAOYSA-N
Formula:	C24H41NO2
SMILES:	CCCCCCCCCCCCCCCCCCCCOC(=O)c1cccnc1
Mol. weight [g/mol]:	375.60

Physical Properties

Property code	Value	Unit	Source
af	1.1278		Cheméo Relay (1.0)
hf	-591.79	kJ/mol	Cheméo Relay (1.0)
hvap	122.86	kJ/mol	Cheméo Relay (1.0)
ie	9.68	eV	Cheméo Relay (1.0)
log10ws	-7.51		Cheméo Relay (1.0)
logp	7.500		Crippen Method
mcvol	342.680	ml/mol	McGowan Method
pc	991.23	kPa	Cheméo Relay (1.0, beta)
rinpol	2846.00		NIST Webbook
tb	659.01	K	Cheméo Relay (1.0)
tc	878.53	K	Cheméo Relay (1.0)
tf	321.16	K	Cheméo Relay (1.0)
vc	1.314	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33233293&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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

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