4-PYRIDINECARBOXYLIC ACID, OCTADECYL ESTER

Other names: Isonicotinic acid, octadecyl ester
Inchi: InChI=1S/C24H41NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-27-24(26)23-18-
InchiKey: VXDJNEIVBJLMMZ-UHFFFAOYSA-N
Formula: C24H41NO2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccncc1
Mol. weight [g/mol]: 375.60

Physical Properties

Property code	Value	Unit	Source
af	1.1296		Cheméo Relay (1.0)
hf	-591.19	kJ/mol	Cheméo Relay (1.0)
hvap	125.07	kJ/mol	Cheméo Relay (1.0)
ie	9.92	eV	Cheméo Relay (1.0)
log10ws	-7.41		Cheméo Relay (1.0)
logp	7.500		Crippen Method
mcvol	342.680	ml/mol	McGowan Method
pc	997.08	kPa	Cheméo Relay (1.0, beta)
rinpol	2817.00		NIST Webbook
tb	658.68	K	Cheméo Relay (1.0)
tc	874.04	K	Cheméo Relay (1.0)
tf	329.83	K	Cheméo Relay (1.0)
vc	1.317	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103225021&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
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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