

Nicotinic acid, heptadecyl ester

Other names:	Nicotinic acid, heptadecyl ester
Inchi:	InChI=1S/C23H39NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-26-23(25)22-18-17-
InchiKey:	NBHWTRRFTRBYCL-UHFFFAOYSA-N
Formula:	C23H39NO2
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)c1cccnc1
Mol. weight [g/mol]:	361.57

Physical Properties

Property code	Value	Unit	Source
af	1.0924		Cheméo Relay (1.0)
hf	-570.60	kJ/mol	Cheméo Relay (1.0)
hvap	118.63	kJ/mol	Cheméo Relay (1.0)
ie	9.65	eV	Cheméo Relay (1.0)
log10ws	-7.21		Cheméo Relay (1.0)
logp	7.110		Crippen Method
mcvol	328.590	ml/mol	McGowan Method
pc	1080.08	kPa	Cheméo Relay (1.0, beta)
rinpol	2752.00		NIST Webbook
tb	652.55	K	Cheméo Relay (1.0)
tc	871.77	K	Cheméo Relay (1.0)
tf	318.61	K	Cheméo Relay (1.0)
vc	1.260	m3/kmol	Cheméo Relay (1.0)

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C862594965&Units=SI

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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