FURFURYLMETHYLAMPHETAMINE

Inchi: InChI=1S/C15H19NO/c1-13(11-14-7-4-3-5-8-14)16(2)12-15-9-6-10-17-15/h3-10,13H,11-
InchiKey: DLGIIZAHQPTVCJ-UHFFFAOYSA-N
Formula: C15H19NO
SMILES: CC(Cc1ccccc1)N(C)Cc1ccco1
Mol. weight [g/mol]: 229.32

Physical Properties

Property code	Value	Unit	Source
af	0.4968		Cheméo Relay (1.0)
hf	52.16	kJ/mol	Cheméo Relay (1.0)
hvap	80.54	kJ/mol	Cheméo Relay (1.0)
ie	7.92	eV	Cheméo Relay (1.0)
log10ws	-1.55		Cheméo Relay (1.0)
logp	3.343		Crippen Method
mcvol	194.840	ml/mol	McGowan Method
pc	2406.73	kPa	Cheméo Relay (1.0, beta)
rinpol	1672.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1672.00		NIST Webbook
ripol	2265.00		NIST Webbook
ripol	2260.00		NIST Webbook
ripol	2273.00		NIST Webbook
ripol	2260.00		NIST Webbook
tb	575.27	K	Cheméo Relay (1.0)
tc	785.17	K	Cheméo Relay (1.0)
tf	288.70	K	Cheméo Relay (1.0)
vc	0.722	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=C13445608&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume