

Moxisylyte

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C16H25NO3/c1-11(2)14-10-15(20-13(4)18)12(3)9-16(14)19-8-7-17(5)6/h9-11H

VRYMTAVOXVTQEF-UHFFFAOYSA-N

C16H25NO3

CC(=O)Oc1cc(C(C)C)c(OCCN(C)C)cc1C

279.38

54-32-0

Physical Properties

Property code	Value	Unit	Source
hfus	35.12	kJ/mol	Joback Method
logp	2.984		Crippen Method
mcvol	235.830	ml/mol	McGowan Method
tf	417.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	3.58720e+01
Coeff. B	1.27832e+00
Coeff. C	-5.86880e-04
Coeff. D	5.50000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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