farmocaine

Inchi: InChI=1S/C17H28N2O2/c1-4-7-12-18-16-10-8-15(9-11-16)17(20)21-14-13-19(5-2)6-3/h8
InchiKey: JQMCLLAJJLVYOC-UHFFFAOYSA-N
Formula: C17H28N2O2
SMILES: CCCCNc1ccc(C(=O)OCCN(CC)CC)cc1
Mol. weight [g/mol]: 292.42

Physical Properties

Property code	Value	Unit	Source
af	0.8493		Cheméo Relay (1.0)
hfus	45.93	kJ/mol	Joback Method
ie	7.40	eV	Cheméo Relay (1.0)
log10ws	-3.51		Cheméo Relay (1.0)
logp	3.397		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
rinpol	2350.00		NIST Webbook
rinpol	2375.00		NIST Webbook
tb	635.85	K	Cheméo Relay (1.0)
tc	832.03	K	Cheméo Relay (1.0)
tf	299.33	K	Cheméo Relay (1.0)
vc	0.914	m3/kmol	Cheméo Relay (1.0)

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	-1.86630e+01
Coeff. B	1.62576e+00
Coeff. C	-9.31760e-04
Coeff. D	1.82500e-07
Coeff. E	0.00000e+00
Basis	predicted

Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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=C3772427&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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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