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
CAS: 3772-42-7

Physical Properties

Property code	Value	Unit	Source
gf	161.29	kJ/mol	Joback Method
hf	-292.95	kJ/mol	Joback Method
hfus	44.34	kJ/mol	Joback Method
hvap	74.01	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.397		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	2350.00		NIST Webbook
rinpol	2375.00		NIST Webbook
tb	758.92	K	Joback Method
tc	953.78	K	Joback Method
tf	477.58	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.37	J/mol×K	758.92	Joback Method
cpg	772.13	J/mol×K	791.40	Joback Method
cpg	787.88	J/mol×K	823.87	Joback Method
cpg	802.66	J/mol×K	856.35	Joback Method
cpg	816.50	J/mol×K	888.83	Joback Method
cpg	829.43	J/mol×K	921.31	Joback Method
cpg	841.50	J/mol×K	953.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3772427&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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