stadacaine

Inchi: InChI=1S/C17H27NO3/c1-4-7-13-20-16-10-8-15(9-11-16)17(19)21-14-12-18(5-2)6-3/h8-1
InchiKey: QNIUOGIMJWORNZ-UHFFFAOYSA-N
Formula: C17H27NO3
SMILES: CCCCOc1ccc(C(=O)OCCN(CC)CC)cc1
Mol. weight [g/mol]: 293.41

Physical Properties

Property code	Value	Unit	Source
gf	-33.10	kJ/mol	Joback Method
hf	-478.64	kJ/mol	Joback Method
hfus	40.43	kJ/mol	Joback Method
hvap	69.98	kJ/mol	Joback Method
log10ws	-3.84		Aqueous Solubility Prediction Method
logp	3.364		Crippen Method
mcvol	249.920	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
tb	731.17	K	Joback Method
tc	923.38	K	Joback Method
tf	447.15	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.80	J/mol×K	731.17	Joback Method
cpg	741.89	J/mol×K	763.20	Joback Method
cpg	757.99	J/mol×K	795.24	Joback Method
cpg	773.12	J/mol×K	827.27	Joback Method
cpg	787.30	J/mol×K	859.31	Joback Method
cpg	800.54	J/mol×K	891.34	Joback Method
cpg	812.89	J/mol×K	923.38	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume