Oxethazaine

Inchi: InChI=1S/C28H41N3O3/c1-27(2,19-23-13-9-7-10-14-23)29(5)25(33)21-31(17-18-32)22-2
InchiKey: FTLDJPRFCGDUFH-UHFFFAOYSA-N
Formula: C28H41N3O3
SMILES: CN(C(=O)CN(CCO)CC(=O)N(C)C(C)(C)Cc1ccccc1)C(C)(C)Cc1ccccc1
Mol. weight [g/mol]: 467.64

Physical Properties

Property code	Value	Unit	Source
gf	353.06	kJ/mol	Joback Method
hf	-340.49	kJ/mol	Joback Method
hfus	57.88	kJ/mol	Joback Method
hvap	116.18	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.240		Crippen Method
mcvol	396.810	ml/mol	McGowan Method
pc	1115.57	kPa	Joback Method
rinpol	2525.00		NIST Webbook
tb	1124.18	K	Joback Method
tc	1379.05	K	Joback Method
tf	721.09	K	Joback Method
vc	1.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1397.72	J/mol×K	1124.18	Joback Method
cpg	1415.90	J/mol×K	1166.66	Joback Method
cpg	1433.85	J/mol×K	1209.14	Joback Method
cpg	1451.86	J/mol×K	1251.62	Joback Method
cpg	1470.21	J/mol×K	1294.10	Joback Method
cpg	1489.19	J/mol×K	1336.57	Joback Method
cpg	1509.08	J/mol×K	1379.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R593578&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