Antazoline, hydroxy-methoxy, hydrolized, acetylated

Inchi: InChI=1S/C22H27N3O5/c1-16(26)23-11-12-24-22(28)15-25(14-18-7-5-4-6-8-18)19-9-10-

InchiKey: LQUPSNUMIFUTGH-UHFFFAOYSA-N

Formula: C22H27N3O5

SMILES: COc1cc(N(CC(=O)NCCNC(C)=O)Cc2ccccc2)ccc1OC(C)=O

Mol. weight [g/mol]: 413.47

Physical Properties

Property code	Value	Unit	Source
gf	32.72	kJ/mol	Joback Method
hf	-475.00	kJ/mol	Joback Method
hfus	60.43	kJ/mol	Joback Method
hvap	110.42	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	1.879		Crippen Method
mcvol	319.710	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tb	1085.31	K	Joback Method
tc	1329.27	K	Joback Method
tf	747.62	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1052.22	J/mol×K	1085.31	Joback Method
cpg	1061.77	J/mol×K	1125.97	Joback Method
cpg	1069.85	J/mol×K	1166.63	Joback Method
cpg	1076.52	J/mol×K	1207.29	Joback Method
cpg	1081.84	J/mol×K	1247.95	Joback Method
cpg	1085.90	J/mol×K	1288.61	Joback Method
cpg	1088.77	J/mol×K	1329.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R536035&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