Antazoline, hydroxy, hydrolized, acetylated

Inchi: InChI=1S/C21H25N3O4/c1-16(25)22-12-13-23-21(27)15-24(14-18-6-4-3-5-7-18)19-8-10-
InchiKey: DTNUXASCFOWTBD-UHFFFAOYSA-N
Formula: C21H25N3O4
SMILES: CC(=O)NCCNC(=O)CN(Cc1ccccc1)c1ccc(OC(C)=O)cc1
Mol. weight [g/mol]: 383.44

Physical Properties

Property code	Value	Unit	Source
gf	138.93	kJ/mol	Joback Method
hf	-310.67	kJ/mol	Joback Method
hfus	57.04	kJ/mol	Joback Method
hvap	105.12	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	1.871		Crippen Method
mcvol	299.750	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2340.00		NIST Webbook
tb	1035.03	K	Joback Method
tc	1271.93	K	Joback Method
tf	701.60	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.74	J/mol×K	1035.03	Joback Method
cpg	981.64	J/mol×K	1074.51	Joback Method
cpg	991.36	J/mol×K	1114.00	Joback Method
cpg	999.98	J/mol×K	1153.48	Joback Method
cpg	1007.60	J/mol×K	1192.96	Joback Method
cpg	1014.31	J/mol×K	1232.45	Joback Method
cpg	1020.19	J/mol×K	1271.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R536020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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