

Antazoline, hydrolized, acetylated

Inchi:	InChI=1S/C19H23N3O2/c1-16(23)20-12-13-21-19(24)15-22(18-10-6-3-7-11-18)14-17-8-4
InchiKey:	QJYCWNIEOSWHAH-UHFFFAOYSA-N
Formula:	C19H23N3O2
SMILES:	CC(=O)NCCNC(=O)CN(Cc1cccc1)c1cccc1
Mol. weight [g/mol]:	325.40

Physical Properties

Property code	Value	Unit	Source
gf	365.64	kJ/mol	Joback Method
hf	-13.12	kJ/mol	Joback Method
hfus	49.46	kJ/mol	Joback Method
hvap	90.85	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	1.946		Crippen Method
mcvol	264.130	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	908.00	K	Joback Method
tc	1135.24	K	Joback Method
tf	594.38	K	Joback Method
vc	0.984	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.69	J/molxK	908.00	Joback Method
cpg	835.07	J/molxK	945.87	Joback Method
cpg	847.38	J/molxK	983.75	Joback Method
cpg	858.71	J/molxK	1021.62	Joback Method
cpg	869.16	J/molxK	1059.50	Joback Method
cpg	878.83	J/molxK	1097.37	Joback Method
cpg	887.83	J/molxK	1135.24	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R536015&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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