

17-Thiosemicarbazonoandrost-5-en-3beta-ol

Inchi: InChI=1S/C20H31N3OS/c1-19-9-7-13(24)11-12(19)3-4-14-15-5-6-17(22-23-18(21)25)20
InchiKey: MOQTVGQHEGMMDS-OQKWZONESA-N
Formula: C20H31N3OS
SMILES: CC12CCC(O)CC1=CCC1C2CCC2(C)C(=NNC(N)=S)CCC12
Mol. weight [g/mol]: 361.55
CAS: 65628-35-5

Physical Properties

Property code	Value	Unit	Source
hf	-37.06	kJ/mol	Joback Method
hvap	103.29	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	3.499		Crippen Method
mcvol	288.480	ml/mol	McGowan Method
pc	1854.71	kPa	Joback Method
tb	1064.67	K	Joback Method
tc	1320.71	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C65628355&Units=SI>
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>

Legend

hf: Enthalpy of formation 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

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