5«alpha»-Androstan-3-one, MO, # 2

Inchi: InChI=1S/C20H33NO/c1-19-10-4-5-17(19)16-7-6-14-13-15(21-22-3)8-12-20(14,2)18(16)9
InchiKey: UYYQSOHBNGRNDB-CWTBSWCASA-N
Formula: C20H33NO
SMILES: CON=C1CCC2(C)C(CCC3C4CCCC4(C)CCC32)C1
Mol. weight [g/mol]: 303.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.56		Cheméo Relay (1.0)
logp	5.422		Crippen Method
mcvol	260.770	ml/mol	McGowan Method
rinpol	2289.00		NIST Webbook
rinpol	2289.00		NIST Webbook
tf	381.12	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R523321&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

tf: Normal melting (fusion) point