

5B-Estran-3-on-17B-ol

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C18H28O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20

RHVBIEJVJWNXBU-UQMVRIFTA-N

C18H28O2

CC12CCC3C4CCC(=O)CC4CCC3C1CCC2O

276.41

Physical Properties

Property code	Value	Unit	Source
gf	-4.85	kJ/mol	Joback Method
hf	-490.16	kJ/mol	Joback Method
hfus	24.93	kJ/mol	Joback Method
hvap	75.02	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.569		Crippen Method
mcvol	228.480	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	2415.00		NIST Webbook
tb	805.78	K	Joback Method
tc	1036.50	K	Joback Method
tf	487.00	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.75	J/mol×K	805.78	Joback Method
cpg	836.59	J/mol×K	844.23	Joback Method
cpg	858.43	J/mol×K	882.69	Joback Method
cpg	879.47	J/mol×K	921.14	Joback Method
cpg	899.90	J/mol×K	959.59	Joback Method
cpg	919.91	J/mol×K	998.05	Joback Method
cpg	939.69	J/mol×K	1036.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R5624&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

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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