

Gona-1,3,5(10)-trien-17-one, 3-methoxy-, (13«alpha»)-

Other names:

13«alpha»-Gona-1,3,5(10)-trien-17-one, 3-methoxy-
3-Methoxy-13-«alpha»-gona-1,3,5(10)-trien-17-one
3-Methoxygona-1,3,5(10)-trien-17-one, (13«alpha»)-

Inchi:

InChI=1S/C18H22O2/c1-20-12-3-5-13-11(10-12)2-4-15-14(13)6-7-17-16(15)8-9-18(17)19

InchiKey:

GDDDQTOBTQTTJD-GZUIOVLMSA-N

Formula:

C18H22O2

SMILES:

COc1ccc2c(c1)CCC1C2CCC2C(=O)CCC21

Mol. weight [g/mol]:

270.37

CAS:

4248-04-8

Physical Properties

Property code	Value	Unit	Source
gf	116.58	kJ/mol	Joback Method
hf	-285.44	kJ/mol	Joback Method
hfus	27.61	kJ/mol	Joback Method
hvap	65.69	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.730		Crippen Method
mcvol	215.580	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
tb	762.21	K	Joback Method
tc	1008.42	K	Joback Method
tf	477.07	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.38	J/molxK	762.21	Joback Method
cpg	709.57	J/molxK	803.24	Joback Method
cpg	729.15	J/molxK	844.28	Joback Method
cpg	747.21	J/molxK	885.31	Joback Method
cpg	763.85	J/molxK	926.35	Joback Method
cpg	779.15	J/molxK	967.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4248048&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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