10A,12a-dimethyl-3,4,4a,5,6,9,10,10a,10b,11,12,12

Inchi: InChI=1S/C19H26O3/c1-18-9-7-13(20)11-12(18)3-4-14-15(18)8-10-19(2)16(14)5-6-17(21

InchiKey: CNIXJDVUMXTEKX-UHFFFAOYSA-N

Formula: C19H26O3

SMILES: CC12CCC3C(CCC4=CC(=O)CCC43C)C1CCC(=O)O2

Mol. weight [g/mol]: 302.41

Physical Properties

Property code	Value	Unit	Source
gf	-50.16	kJ/mol	Joback Method
hf	-532.20	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	69.92	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.814		Crippen Method
mcvol	239.840	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
tb	849.24	K	Joback Method
tc	1118.73	K	Joback Method
tf	574.38	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.60	J/mol×K	849.24	Joback Method
cpg	870.50	J/mol×K	894.16	Joback Method
cpg	897.23	J/mol×K	939.07	Joback Method
cpg	924.19	J/mol×K	983.99	Joback Method
cpg	951.80	J/mol×K	1028.90	Joback Method
cpg	980.45	J/mol×K	1073.82	Joback Method
cpg	1010.56	J/mol×K	1118.73	Joback Method

Sources

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=B6005438&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume