(+)«beta»-Desmotroposantonin methyl ether

Inchi: InChI=1S/C16H20O3/c1-8-7-13(18-4)10(3)14-11(8)5-6-12-9(2)16(17)19-15(12)14/h7,9,1
InchiKey: GNCNKCJJKNUKGL-UHFFFAOYSA-N
Formula: C16H20O3
SMILES: COc1cc(C)c2c(c1C)C1OC(=O)C(C)C1CC2
Mol. weight [g/mol]: 260.33
CAS: 1693-61-4

Physical Properties

Property code	Value	Unit	Source
chs	-8486.30 ± 1.90	kJ/mol	NIST Webbook
gf	-54.29	kJ/mol	Joback Method
hf	-465.74	kJ/mol	Joback Method
hfs	-668.20 ± 1.90	kJ/mol	NIST Webbook
hfus	33.60	kJ/mol	Joback Method
hvap	66.99	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.108		Crippen Method
mcvol	204.130	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
tb	742.35	K	Joback Method
tc	974.63	K	Joback Method
tf	491.72	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.39	J/mol×K	742.35	Joback Method
cpg	637.81	J/mol×K	781.06	Joback Method
cpg	654.98	J/mol×K	819.78	Joback Method
cpg	670.93	J/mol×K	858.49	Joback Method
cpg	685.67	J/mol×K	897.20	Joback Method
cpg	699.23	J/mol×K	935.92	Joback Method
cpg	711.64	J/mol×K	974.63	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=C1693614&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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