(+)«beta»-Desmotroposantonin acetate

Inchi:	InChI=1S/C17H20O4/c1-8-7-14(20-11(4)18)10(3)15-12(8)5-6-13-9(2)17(19)21-16(13)15/
InchiKey:	ZWPKGSNVVQTUMS-UHFFFAOYSA-N
Formula:	C17H20O4
SMILES:	CC(=O)Oc1cc(C)c2c(c1C)C1OC(=O)C(C)C1CC2
Mol. weight [g/mol]:	288.34
CAS:	14794-69-5

Physical Properties

Property code	Value	Unit	Source
chs	-8668.70 ± 1.80	kJ/mol	NIST Webbook
gf	-174.79	kJ/mol	Joback Method
hf	-598.96	kJ/mol	Joback Method
hfs	-879.30 ± 1.80	kJ/mol	NIST Webbook
hfus	37.79	kJ/mol	Joback Method
hvap	75.96	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.025		Crippen Method
mcvol	219.790	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
tb	819.10	K	Joback Method
tc	1052.72	K	Joback Method
tf	552.92	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.64	J/mol×K	819.10	Joback Method
cpg	710.21	J/mol×K	858.04	Joback Method
cpg	725.48	J/mol×K	896.97	Joback Method
cpg	739.46	J/mol×K	935.91	Joback Method
cpg	752.20	J/mol×K	974.85	Joback Method
cpg	763.71	J/mol×K	1013.79	Joback Method
cpg	774.01	J/mol×K	1052.72	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=C14794695&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

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