Kessoglycyl monoacetate

Inchi: InChI=1S/C17H28O4/c1-9-6-14(20-10(2)18)15-11(9)7-12-13(19)8-17(15,5)21-16(12,3)4/
InchiKey: KSJYGLBFXLTFDO-UUUUAQTGSA-N
Formula: C17H28O4
SMILES: CC(=O)OC1CC(C)C2CC3C(O)CC(C)(OC3(C)C)C12
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-268.18	kJ/mol	Joback Method
hf	-794.54	kJ/mol	Joback Method
hfus	35.50	kJ/mol	Joback Method
hvap	80.19	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.529		Crippen Method
mcvol	236.990	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	1972.00		NIST Webbook
tb	793.94	K	Joback Method
tc	1004.15	K	Joback Method
tf	510.76	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.96	J/mol×K	793.94	Joback Method
cpg	833.77	J/mol×K	828.97	Joback Method
cpg	854.26	J/mol×K	864.01	Joback Method
cpg	874.64	J/mol×K	899.04	Joback Method
cpg	895.11	J/mol×K	934.08	Joback Method
cpg	915.87	J/mol×K	969.11	Joback Method
cpg	937.14	J/mol×K	1004.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224950&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume