2H-Cyclohepta[b]furan-2-one, 6-[1-(acetyloxy)-3-oxobutyl]-3,3a,4,7,8,8a-hexahyd

Other names:	2H-Cyclohepta[b]furan-2-one, 3,3a,4,7,8,8a-hexahydro-6-(1-hydroxy-3-oxobutyl)-7-methyl-3-methylene-, acetate, (3aR,7S,8aS)- Xanthinin,
Inchi:	InChI=1S/C17H22O5/c1-9-7-15-14(11(3)17(20)22-15)6-5-13(9)16(8-10(2)18)21-12(4)19/
InchiKey:	DPSCQKGSAHTWSP-UHFFFAOYSA-N
Formula:	C17H22O5
SMILES:	C=C1C(=O)OC2CC(C)C(C(CC(C)=O)OC(C)=O)=CCC12
Mol. weight [g/mol]:	306.35
CAS:	580-49-4

Physical Properties

Property code	Value	Unit	Source
gf	-342.93	kJ/mol	Joback Method
hf	-795.40	kJ/mol	Joback Method
hfus	36.75	kJ/mol	Joback Method
hvap	79.03	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.351		Crippen Method
mcvol	236.520	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	2383.00		NIST Webbook
rinpol	2383.00		NIST Webbook
tb	842.04	K	Joback Method
tc	1068.34	K	Joback Method
tf	527.75	K	Joback Method
vc	0.890	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.73	J/mol×K	842.04	Joback Method
cpg	777.84	J/mol×K	879.76	Joback Method
cpg	792.44	J/mol×K	917.47	Joback Method
cpg	805.53	J/mol×K	955.19	Joback Method
cpg	817.10	J/mol×K	992.91	Joback Method

cpg	827.14	J/mol×K	1030.62	Joback Method
cpg	835.67	J/mol×K	1068.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C580494&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

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

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