

(S,E)-4-Hydroxy-3,5,5-trimethyl-4-(3-oxobut-1-en-1

Inchi:	InChI=1S/C13H18O3/c1-9-7-11(15)8-12(3,4)13(9,16)6-5-10(2)14/h5-7,16H,8H2,1-4H3/b
InchiKey:	JJRYPMXNLLZFH-GFUIURDCSA-N
Formula:	C13H18O3
SMILES:	CC(=O)C=CC1(O)C(C)=CC(=O)CC1(C)C
Mol. weight [g/mol]:	222.28
CAS:	39763-33-2

Physical Properties

Property code	Value	Unit	Source
gf	-223.44	kJ/mol	Joback Method
hf	-486.17	kJ/mol	Joback Method
hfus	15.97	kJ/mol	Joback Method
hvap	70.93	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	1.808		Crippen Method
mvol	183.580	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1799.80		NIST Webbook
rinpol	1799.80		NIST Webbook
tb	734.37	K	Joback Method
tc	955.11	K	Joback Method
tf	474.38	K	Joback Method
vc	0.690	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.71	J/molxK	734.37	Joback Method
cpg	540.92	J/molxK	771.16	Joback Method
cpg	555.92	J/molxK	807.95	Joback Method
cpg	570.90	J/molxK	844.74	Joback Method
cpg	586.06	J/molxK	881.53	Joback Method
cpg	601.58	J/molxK	918.32	Joback Method
cpg	617.66	J/molxK	955.11	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=C39763332&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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