Cinnamic acid, alpha-acetyl-4-hydroxy-beta-(hydroxymethyl)-3-m

Inchi: InChI=1S/C13H12O5/c1-7(14)12-9(6-18-13(12)16)8-3-4-10(15)11(5-8)17-2/h3-5,15H,6H

InchiKey: ULTWKORORDEMCL-UHFFFAOYSA-N

Formula: C13H12O5

SMILES: COc1cc(C2=C(C(C)=O)C(=O)OC2)ccc1O

Mol. weight [g/mol]: 248.23

CAS: 73839-65-3

Physical Properties

Property code	Value	Unit	Source
gf	-380.93	kJ/mol	Joback Method
hf	-662.74	kJ/mol	Joback Method
hfus	32.45	kJ/mol	Joback Method
hvap	80.58	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.300		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
tb	809.25	K	Joback Method
tc	1060.13	K	Joback Method
tf	594.82	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.31	J/mol×K	809.25	Joback Method
cpg	519.60	J/mol×K	851.06	Joback Method
cpg	530.98	J/mol×K	892.88	Joback Method
cpg	541.49	J/mol×K	934.69	Joback Method
cpg	551.18	J/mol×K	976.50	Joback Method
cpg	560.11	J/mol×K	1018.31	Joback Method
cpg	568.32	J/mol×K	1060.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73839653&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume