3-Acetoxycinnamic acid

Other names: m-Acetyl coumaric acid
Inchi: InChI=1S/C11H10O4/c1-8(12)15-10-4-2-3-9(7-10)5-6-11(13)14/h2-7H,1H3,(H,13,14)/b6-
InchiKey: LSZKRNUEKNCZIE-AATRIKPKSA-N
Formula: C11H10O4
SMILES: CC(=O)Oc1cccc(C=CC(=O)O)c1
Mol. weight [g/mol]: 206.19
CAS: 20375-42-2

Physical Properties

Property code	Value	Unit	Source
chs	-5062.51	kJ/mol	NIST Webbook
gf	-274.92	kJ/mol	Joback Method
hf	-437.70	kJ/mol	Joback Method
hfus	26.57	kJ/mol	Joback Method
hvap	75.56	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.710		Crippen Method
mcvol	152.670	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
tb	709.24	K	Joback Method
tc	920.04	K	Joback Method
tf	430.50	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.59	J/mol×K	709.24	Joback Method
cpg	397.35	J/mol×K	744.37	Joback Method
cpg	406.43	J/mol×K	779.51	Joback Method
cpg	414.87	J/mol×K	814.64	Joback Method
cpg	422.70	J/mol×K	849.77	Joback Method
cpg	429.94	J/mol×K	884.90	Joback Method
cpg	436.63	J/mol×K	920.04	Joback Method

dvisc	0.0011697	Pa×s	430.50	Joback Method
dvisc	0.0005135	Pa×s	476.96	Joback Method
dvisc	0.0002609	Pa×s	523.41	Joback Method
dvisc	0.0001480	Pa×s	569.87	Joback Method
dvisc	0.0000915	Pa×s	616.33	Joback Method
dvisc	0.0000605	Pa×s	662.78	Joback Method
dvisc	0.0000422	Pa×s	709.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20375422&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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