

3-Acetoxyacinnamic 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:	LSZKRNUKNCZIE-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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

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

Sources

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=C20375422&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

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

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