o-Acetoxycinnamic acid

Other names:	2-Acetoxycinnamic acid
	O-Acetyl-O-coumaric acid
	Tylmarin
	2-Propenoic acid, 3-(2-(acetyloxy)phenyl)-
	Cinnamic acid, 2-acetoxy-
	3-[2-(Acetyloxy)phenyl]-2-propenoic acid
Inchi:	InChI=1S/C11H10O4/c1-8(12)15-10-5-3-2-4-9(10)6-7-11(13)14/h2-7H,1H3,(H,13,14)/b7-
InchiKey:	UXOWQQCLBQBRMQ-VOTSOKGWSA-N
Formula:	C11H10O4
SMILES:	CC(=O)Oc1ccccc1C=CC(=O)O
Mol. weight [g/mol]:	206.19
CAS:	55620-18-3

Physical Properties

Property code	Value	Unit	Source
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	429.94	J/mol×K	884.90	Joback Method
cpg	422.70	J/mol×K	849.77	Joback Method

cpg	414.87	J/mol×K	814.64	Joback Method
cpg	406.43	J/mol×K	779.51	Joback Method
cpg	397.35	J/mol×K	744.37	Joback Method
cpg	436.63	J/mol×K	920.04	Joback Method
dvisc	0.0000422	Pa×s	709.24	Joback Method
dvisc	0.0000605	Pa×s	662.78	Joback Method
dvisc	0.0000915	Pa×s	616.33	Joback Method
dvisc	0.0001480	Pa×s	569.87	Joback Method
dvisc	0.0002609	Pa×s	523.41	Joback Method
dvisc	0.0005135	Pa×s	476.96	Joback Method
dvisc	0.0011697	Pa×s	430.50	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55620183&Units=SI

Legend

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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