Acetic acid, 2-methylphenyl ester

Other names:	Acetic acid, o-tolyl ester
	o-Acetoxytoluene
	o-Cresol acetate
	o-Cresyl acetate
	o-Cresylic acetate
	o-Methylphenyl acetate
	o-Tolyl acetate
	Acetyl-o-cresol
	2-Methylphenyl acetate
	2-Methylphenyl ester of acetic acid
	2-Acetoxytoluene
	NSC 58961
Inchi:	InChI=1S/C9H10O2/c1-7-5-3-4-6-9(7)11-8(2)10/h3-6H,1-2H3
InchiKey:	AMZORBZSQRUXNC-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	CC(=O)Oc1ccccc1C
Mol. weight [g/mol]:	150.17
CAS:	533-18-6

Physical Properties

Property code	Value	Unit	Source
gf	-106.24	kJ/mol	Joback Method
hf	-248.83	kJ/mol	Joback Method
hfus	15.50	kJ/mol	Joback Method
hvap	47.72	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
ie	8.38 ± 0.02	eV	NIST Webbook
log10ws	-2.26		Crippen Method
logp	1.920		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	1111.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1122.00		NIST Webbook
ripol	1716.00		NIST Webbook
ripol	1716.00		NIST Webbook
tb	481.20	K	NIST Webbook

tc	730.64	K	Joback Method
tf	302.29	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.24	J/mol×K	513.27	Joback Method
cpg	268.48	J/mol×K	549.50	Joback Method
cpg	280.07	J/mol×K	585.73	Joback Method
cpg	291.03	J/mol×K	621.95	Joback Method
cpg	301.35	J/mol×K	658.18	Joback Method
cpg	311.06	J/mol×K	694.41	Joback Method
cpg	320.16	J/mol×K	730.64	Joback Method
dvisc	0.0017319	Pa×s	302.29	Joback Method
dvisc	0.0010297	Pa×s	337.45	Joback Method
dvisc	0.0006754	Pa×s	372.62	Joback Method
dvisc	0.0004764	Pa×s	407.78	Joback Method
dvisc	0.0003552	Pa×s	442.94	Joback Method
dvisc	0.0002765	Pa×s	478.11	Joback Method
dvisc	0.0002227	Pa×s	513.27	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C533186&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
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume