Acetic acid, 4-methylphenyl ester

Other names:	Acetic acid, p-tolyl ester
	p-Acetoxytoluene
	p-Cresol acetate
	p-Cresyl acetate
	p-Methylphenyl acetate
	p-Tolyl acetate
	p-Tolyl ethanoate
	Narceol
	4-Acetoxytoluene
	4-Methylphenyl acetate
	Cresyl acetate
	4-Tolyl acetate
	Paracresyl acetate
	p-Cresylic acetate
	NSC 43244
Inchi:	InChI=1S/C9H10O2/c1-7-3-5-9(6-4-7)11-8(2)10/h3-6H,1-2H3
InchiKey:	CDJJKTLOZJAGIZ-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	CC(=O)Oc1ccc(C)cc1
Mol. weight [g/mol]:	150.17
CAS:	140-39-6

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	8.60 ± 0.20	eV	NIST Webbook
ie	7.84 ± 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	1135.90		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1142.00		NIST Webbook

rinpol	1150.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1142.40		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1136.50		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1171.40		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1722.30		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1722.90		NIST Webbook
tb	483.70	K	NIST Webbook
tb	485.70	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	320.16	J/mol×K	730.64	Joback Method
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
dvisc	0.0002227	Pa×s	513.27	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
hvapt	55.90	kJ/mol	432.50	NIST Webbook

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=C140396&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
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

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