2,6-Dimethylphenyl acetate

Inchi: InChI=1S/C10H12O2/c1-7-5-4-6-8(2)10(7)12-9(3)11/h4-6H,1-3H3
InchiKey: UDDBRJGGGUMTQZ-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CC(=O)Oc1c(C)cccc1C
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
gf	-107.45	kJ/mol	Joback Method
hf	-280.94	kJ/mol	Joback Method
hfus	17.71	kJ/mol	Joback Method
hvap	50.61	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.229		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1211.00		NIST Webbook
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tb	541.13	K	Joback Method
tc	756.04	K	Joback Method
tf	326.08	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.97	J/mol×K	541.13	Joback Method
cpg	358.27	J/mol×K	720.22	Joback Method
cpg	347.89	J/mol×K	684.40	Joback Method
cpg	336.88	J/mol×K	648.58	Joback Method
cpg	325.22	J/mol×K	612.77	Joback Method
cpg	312.92	J/mol×K	576.95	Joback Method
cpg	368.03	J/mol×K	756.04	Joback Method
dvisc	0.0002040	Pa×s	541.13	Joback Method

dvisc	0.0002500	Pa×s	505.29	Joback Method
dvisc	0.0003161	Pa×s	469.45	Joback Method
dvisc	0.0004153	Pa×s	433.61	Joback Method
dvisc	0.0005733	Pa×s	397.76	Joback Method
dvisc	0.0008436	Pa×s	361.92	Joback Method
dvisc	0.0013513	Pa×s	326.08	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=U373478&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume