Acetic acid, (2,4-xylyl)-

Other names:	2,4-Dimethylphenylacetic acid
Inchi:	InChI=1S/C10H12O2/c1-7-3-4-9(6-10(11)12)8(2)5-7/h3-5H,6H2,1-2H3,(H,11,12)
InchiKey:	MWBXCWLRASBZFB-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	Cc1ccc(CC(=O)O)c(C)c1
Mol. weight [g/mol]:	164.20
CAS:	6331-04-0

Physical Properties

Property code	Value	Unit	Source
chs	-5150.10	kJ/mol	NIST Webbook
gf	-139.27	kJ/mol	Joback Method
hf	-300.95	kJ/mol	Joback Method
hfs	-504.20	kJ/mol	NIST Webbook
hfus	20.61	kJ/mol	Joback Method
hvap	64.88	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	1.931		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
tb	610.89	K	Joback Method
tc	813.03	K	Joback Method
tf	364.67	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.71	J/mol×K	610.89	Joback Method
cpg	374.26	J/mol×K	779.34	Joback Method
cpg	365.68	J/mol×K	745.65	Joback Method
cpg	356.56	J/mol×K	711.96	Joback Method
cpg	346.86	J/mol×K	678.27	Joback Method
cpg	336.59	J/mol×K	644.58	Joback Method

cpg	382.32	J/mol×K	813.03	Joback Method
dvisc	0.0000861	Pa×s	610.89	Joback Method
dvisc	0.0001247	Pa×s	569.85	Joback Method
dvisc	0.0001915	Pa×s	528.82	Joback Method
dvisc	0.0003160	Pa×s	487.78	Joback Method
dvisc	0.0005718	Pa×s	446.74	Joback Method
dvisc	0.0011664	Pa×s	405.71	Joback Method
dvisc	0.0027935	Pa×s	364.67	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=C6331040&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfs:	Solid phase 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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