

Acetylvanillone

Inchi:	InChI=1S/C9H10O3/c1-6(10)7-3-4-8(11)9(5-7)12-2/h3-5,11H,1-2H3
InchiKey:	DFYRUELUNQRZTB-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COc1cc(C(C)=O)ccc1O
Mol. weight [g/mol]:	166.17

Physical Properties

Property code	Value	Unit	Source
gf	-260.86	kJ/mol	Joback Method
hf	-426.14	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	60.74	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.603		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
rinpol	1494.00		NIST Webbook
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tb	593.89	K	Joback Method
tc	822.63	K	Joback Method
tf	414.01	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.95	J/mol×K	593.89	Joback Method
cpg	313.95	J/mol×K	632.01	Joback Method
cpg	324.24	J/mol×K	670.14	Joback Method
cpg	333.88	J/mol×K	708.26	Joback Method
cpg	342.92	J/mol×K	746.38	Joback Method
cpg	351.43	J/mol×K	784.51	Joback Method
cpg	359.45	J/mol×K	822.63	Joback Method
dvisc	0.0007214	Pa×s	414.01	Joback Method

dvisc	0.0003744	Pa×s	443.99	Joback Method
dvisc	0.0002111	Pa×s	473.97	Joback Method
dvisc	0.0001274	Pa×s	503.95	Joback Method
dvisc	0.0000814	Pa×s	533.93	Joback Method
dvisc	0.0000546	Pa×s	563.91	Joback Method
dvisc	0.0000381	Pa×s	593.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R614843&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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