2-methylpropiovanillone

Inchi: InChI=1S/C11H14O3/c1-4-9(12)8-5-6-10(13)11(14-3)7(8)2/h5-6,13H,4H2,1-3H3
InchiKey: ITMQIDBFFCXSCX-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CCC(=O)c1ccc(O)c(OC)c1C
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
gf	-253.65	kJ/mol	Joback Method
hf	-478.89	kJ/mol	Joback Method
hfus	26.08	kJ/mol	Joback Method
hvap	65.85	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.302		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
rinpol	1611.00		NIST Webbook
rinpol	1611.00		NIST Webbook
tb	644.63	K	Joback Method
tc	865.86	K	Joback Method
tf	449.07	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.40	J/mol×K	644.63	Joback Method
cpg	408.86	J/mol×K	681.50	Joback Method
cpg	420.62	J/mol×K	718.37	Joback Method
cpg	431.71	J/mol×K	755.24	Joback Method
cpg	442.19	J/mol×K	792.11	Joback Method
cpg	452.10	J/mol×K	828.99	Joback Method
cpg	461.50	J/mol×K	865.86	Joback Method
dvisc	0.0003955	Pa×s	449.07	Joback Method

dvisc	0.0002113	Pa×s	481.66	Joback Method
dvisc	0.0001223	Pa×s	514.26	Joback Method
dvisc	0.0000755	Pa×s	546.85	Joback Method
dvisc	0.0000492	Pa×s	579.44	Joback Method
dvisc	0.0000336	Pa×s	612.04	Joback Method
dvisc	0.0000238	Pa×s	644.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R490845&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

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