Butyrovanillone

Inchi: InChI=1S/C11H14O3/c1-3-4-9(12)8-5-6-10(13)11(7-8)14-2/h5-7,13H,3-4H2,1-2H3
InchiKey: ATFSJFVUBBVFDB-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CCCC(=O)c1ccc(O)c(OC)c1
Mol. weight [g/mol]: 194.23
CAS: 64142-23-0

Physical Properties

Property code	Value	Unit	Source
gf	-244.02	kJ/mol	Joback Method
hf	-467.42	kJ/mol	Joback Method
hfus	26.47	kJ/mol	Joback Method
hvap	65.19	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.384		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
rinpol	1592.00		NIST Webbook
rinpol	1592.00		NIST Webbook
ripol	2771.00		NIST Webbook
ripol	2771.00		NIST Webbook
tb	639.65	K	Joback Method
tc	859.98	K	Joback Method
tf	436.55	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.49	J/mol×K	639.65	Joback Method
cpg	453.72	J/mol×K	823.26	Joback Method
cpg	443.76	J/mol×K	786.54	Joback Method
cpg	433.22	J/mol×K	749.81	Joback Method
cpg	422.03	J/mol×K	713.09	Joback Method

cpg	410.14	J/mol×K	676.37	Joback Method
cpg	463.15	J/mol×K	859.98	Joback Method
dvisc	0.0000247	Pa×s	639.65	Joback Method
dvisc	0.0000357	Pa×s	605.80	Joback Method
dvisc	0.0000539	Pa×s	571.95	Joback Method
dvisc	0.0000856	Pa×s	538.10	Joback Method
dvisc	0.0001447	Pa×s	504.25	Joback Method
dvisc	0.0002638	Pa×s	470.40	Joback Method
dvisc	0.0005280	Pa×s	436.55	Joback Method

Sources

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=C64142230&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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