Vanillic acid, n-butyl ester

Other names: butyl vanillate
Inchi: InChI=1S/C12H16O4/c1-3-4-7-16-12(14)9-5-6-10(13)11(8-9)15-2/h5-6,8,13H,3-4,7H2,1-2
InchiKey: TUOSEEPBHUCCAO-UHFFFAOYSA-N
Formula: C12H16O4
SMILES: CCCCOC(=O)c1ccc(O)c(OC)c1
Mol. weight [g/mol]: 224.25
CAS: 5348-74-3

Physical Properties

Property code	Value	Unit	Source
gf	-340.60	kJ/mol	Joback Method
hf	-620.28	kJ/mol	Joback Method
hfus	30.25	kJ/mol	Joback Method
hvap	69.82	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.358		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
tb	684.95	K	Joback Method
tc	899.10	K	Joback Method
tf	470.05	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.12	J/mol×K	684.95	Joback Method
cpg	485.23	J/mol×K	720.64	Joback Method
cpg	497.60	J/mol×K	756.33	Joback Method
cpg	509.26	J/mol×K	792.03	Joback Method
cpg	520.25	J/mol×K	827.72	Joback Method
cpg	530.63	J/mol×K	863.41	Joback Method
cpg	540.42	J/mol×K	899.10	Joback Method
dvisc	0.0002706	Pa×s	470.05	Joback Method

dvisc	0.0001389	Pa×s	505.87	Joback Method
dvisc	0.0000779	Pa×s	541.68	Joback Method
dvisc	0.0000469	Pa×s	577.50	Joback Method
dvisc	0.0000300	Pa×s	613.32	Joback Method
dvisc	0.0000201	Pa×s	649.13	Joback Method
dvisc	0.0000141	Pa×s	684.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5348743&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume