3-Buten-2-ol, benzoate

Inchi: InChI=1S/C11H12O2/c1-3-9(2)13-11(12)10-7-5-4-6-8-10/h3-9H,1H2,2H3
InchiKey: ZNWBXXLWBPWQAT-UHFFFAOYSA-N
Formula: C11H12O2
SMILES: C=CC(C)OC(=O)c1ccccc1
Mol. weight [g/mol]: 176.21
CAS: 65001-62-9

Physical Properties

Property code	Value	Unit	Source
gf	5.63	kJ/mol	Joback Method
hf	-158.49	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	50.45	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.418		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
tb	550.29	K	Joback Method
tc	768.70	K	Joback Method
tf	295.55	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.26	J/mol×K	550.29	Joback Method
cpg	389.61	J/mol×K	732.30	Joback Method
cpg	378.77	J/mol×K	695.90	Joback Method
cpg	367.14	J/mol×K	659.49	Joback Method
cpg	354.70	J/mol×K	623.09	Joback Method
cpg	341.42	J/mol×K	586.69	Joback Method
cpg	399.69	J/mol×K	768.70	Joback Method
dvisc	0.0001934	Pa×s	550.29	Joback Method
dvisc	0.0002512	Pa×s	507.83	Joback Method

dvisc	0.0003422	Pa×s	465.38	Joback Method
dvisc	0.0004960	Pa×s	422.92	Joback Method
dvisc	0.0007809	Pa×s	380.46	Joback Method
dvisc	0.0013782	Pa×s	338.01	Joback Method
dvisc	0.0028634	Pa×s	295.55	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=C65001629&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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