

Benzoic acid, 4-hydroxy-, 2-methylbutyl ester

Inchi:	InChI=1S/C12H16O3/c1-3-9(2)8-15-12(14)10-4-6-11(13)7-5-10/h4-7,9,13H,3,8H2,1-2H3
InchiKey:	YCVMFKRVG0AHAA-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	CCC(C)COC(=O)c1ccc(O)cc1
Mol. weight [g/mol]:	208.25

Physical Properties

Property code	Value	Unit	Source
gf	-228.41	kJ/mol	Joback Method
hf	-481.87	kJ/mol	Joback Method
hfus	25.92	kJ/mol	Joback Method
hvap	66.36	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.595		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinsol	1812.00		NIST Webbook
tb	657.11	K	Joback Method
tc	877.01	K	Joback Method
tf	420.30	K	Joback Method
vc	0.584	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.59	J/molxK	657.11	Joback Method
cpg	509.60	J/molxK	840.36	Joback Method
cpg	498.85	J/molxK	803.71	Joback Method
cpg	487.44	J/molxK	767.06	Joback Method
cpg	475.31	J/molxK	730.41	Joback Method
cpg	462.38	J/molxK	693.76	Joback Method
cpg	519.75	J/molxK	877.01	Joback Method
dvisc	0.0000192	Paxs	657.11	Joback Method
dvisc	0.0000294	Paxs	617.64	Joback Method

dvisc	0.0000478	Paxs	578.17	Joback Method
dvisc	0.0000834	Paxs	538.71	Joback Method
dvisc	0.0001589	Paxs	499.24	Joback Method
dvisc	0.0003381	Paxs	459.77	Joback Method
dvisc	0.0008293	Paxs	420.30	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=U375439&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
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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