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

Other names: Salicylic acid, 2-methylbutyl ester
2-methylbutyl salicylate
Inchi: InChI=1S/C12H16O3/c1-3-9(2)8-15-12(14)10-6-4-5-7-11(10)13/h4-7,9,13H,3,8H2,1-2H3
InchiKey: LCMNCRZMVCRJNZ-UHFFFAOYSA-N
Formula: C12H16O3
SMILES: CCC(C)COC(=O)c1ccccc1O
Mol. weight [g/mol]: 208.25
CAS: 51115-63-0

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
rinpol	1509.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1554.00		NIST Webbook
tb	657.11	K	Joback Method
tc	877.01	K	Joback Method
tf	420.30	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.59	J/mol×K	657.11	Joback Method
cpg	462.38	J/mol×K	693.76	Joback Method
cpg	475.31	J/mol×K	730.41	Joback Method
cpg	487.44	J/mol×K	767.06	Joback Method

cpg	498.85	J/mol×K	803.71	Joback Method
cpg	509.60	J/mol×K	840.36	Joback Method
cpg	519.75	J/mol×K	877.01	Joback Method
dvisc	0.0008293	Pa×s	420.30	Joback Method
dvisc	0.0003381	Pa×s	459.77	Joback Method
dvisc	0.0001589	Pa×s	499.24	Joback Method
dvisc	0.0000834	Pa×s	538.71	Joback Method
dvisc	0.0000478	Pa×s	578.17	Joback Method
dvisc	0.0000294	Pa×s	617.64	Joback Method
dvisc	0.0000192	Pa×s	657.11	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51115630&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

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