Isoamyl salicylate

Other names:	3-Methylbutyl 2-hydroxybenzoate
	3-methylbutyl salicylate
	34377-38-3
	Benzoic acid, 2-hydroxy-, 3-methylbutyl ester
	Benzoic acid, o-hydroxy, 3-methylbutyl ester
	Isoamyl o-hydroxybenzoate
	Isoamylester kyseliny salicylove
	Isopentyl salicylate
	Isopentyl-2-hydroxyphenyl methanoate
	NSC 7952
	Orchidee
	Salicylic acid, 3-methylbutyl ester
	Salicylic acid, isopentyl ester
	Sanfoin
Inchi:	InChI=1S/C12H16O3/c1-9(2)7-8-15-12(14)10-5-3-4-6-11(10)13/h3-6,9,13H,7-8H2,1-2H3
InchiKey:	PMGCQNGBLMMXEW-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	CC(C)CCOC(=O)c1ccccc1O
Mol. weight [g/mol]:	208.25
CAS:	87-20-7

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	-3.16		Aqueous Solubility Prediction Method
logp	2.595		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1534.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1542.00		NIST Webbook

rinpol	1515.40		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1506.70		NIST Webbook
rinpol	1505.70		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1515.00		NIST Webbook
ripol	2032.90		NIST Webbook
ripol	2021.00		NIST Webbook
ripol	2035.00		NIST Webbook
ripol	2024.00		NIST Webbook
ripol	2037.10		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	519.75	J/mol×K	877.01	Joback Method
cpg	509.60	J/mol×K	840.36	Joback Method
cpg	498.85	J/mol×K	803.71	Joback Method
cpg	487.44	J/mol×K	767.06	Joback Method
cpg	475.31	J/mol×K	730.41	Joback Method
cpg	462.38	J/mol×K	693.76	Joback Method
cpg	448.59	J/mol×K	657.11	Joback Method
dvisc	0.0008293	Pa×s	420.30	Joback Method
dvisc	0.0000192	Pa×s	657.11	Joback Method
dvisc	0.0000294	Pa×s	617.64	Joback Method
dvisc	0.0000478	Pa×s	578.17	Joback Method
dvisc	0.0000834	Pa×s	538.71	Joback Method
dvisc	0.0001589	Pa×s	499.24	Joback Method
dvisc	0.0003381	Pa×s	459.77	Joback Method
hvapt	73.00	kJ/mol	308.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	424.70	K	2.00	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87207&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume