Phenyl salicylate

Other names:	2-Hydroxy-benzoic acid phenyl ester
	2-Phenoxycarbonylphenol
	2-hydroxybenzoic acid phenyl ester
	Benzoic acid, 2-hydroxy-, phenyl ester
	Fenylester kyseliny salicylove
	Musol
	NSC 33406
	Phenol salicylate
	Phenyl 2-hydroxybenzoate
	Salicylic acid, phenyl ester
	Salol
	Salphenyl
	Seesorb 201
	Seesorb K 201
	phenyl 2-hydroxybenzenecarboxylate
	salicylic acid phenyl ester
Inchi:	InChI=1S/C13H10O3/c14-12-9-5-4-8-11(12)13(15)16-10-6-2-1-3-7-10/h1-9,14H
InchiKey:	ZQBAKBUEJOMQEX-UHFFFAOYSA-N
Formula:	C13H10O3
SMILES:	O=C(Oc1ccccc1)c1ccccc1O
Mol. weight [g/mol]:	214.22
CAS:	118-55-8

Physical Properties

Property code	Value	Unit	Source
chs	-6109.10	kJ/mol	NIST Webbook
gf	-105.14	kJ/mol	Joback Method
hf	-260.70	kJ/mol	Joback Method
hfus	26.08	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-3.15		Aqueous Solubility Prediction Method
logp	2.611		Crippen Method
mcvol	159.820	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
rinpol	1650.00		NIST Webbook
rinpol	1702.00		NIST Webbook

rinpol	1655.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1702.00		NIST Webbook
tb	707.11	K	Joback Method
tc	962.79	K	Joback Method
tf	314.90	K	The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters
tf	314.83 ± 0.25	K	NIST Webbook
tf	315.00 ± 1.50	K	NIST Webbook
tf	314.53 ± 1.00	K	NIST Webbook
tf	314.49 ± 0.20	K	NIST Webbook
tf	314.82 ± 0.20	K	NIST Webbook
tf	314.84 ± 0.20	K	NIST Webbook
tt	314.75	K	Investigation of the melting behavior of the reference materials biphenyl and phenyl salicylate by a new type adiabatic scanning calorimeter
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.02	J/mol×K	920.18	Joback Method
cpg	475.68	J/mol×K	962.79	Joback Method
cpg	413.44	J/mol×K	707.11	Joback Method
cpg	425.94	J/mol×K	749.72	Joback Method
cpg	437.42	J/mol×K	792.34	Joback Method
cpg	448.02	J/mol×K	834.95	Joback Method
cpg	457.84	J/mol×K	877.56	Joback Method
dvisc	0.0000213	Pa×s	668.09	Joback Method
dvisc	0.0000147	Pa×s	707.11	Joback Method
dvisc	0.0003388	Pa×s	472.99	Joback Method
dvisc	0.0001645	Pa×s	512.01	Joback Method
dvisc	0.0000885	Pa×s	551.03	Joback Method
dvisc	0.0000517	Pa×s	590.05	Joback Method

dvisc	0.0000323	Pa×s	629.07	Joback Method
hfust	18.98	kJ/mol	314.20	NIST Webbook
hfust	19.16	kJ/mol	315.00	NIST Webbook
hfust	19.20	kJ/mol	315.10	NIST Webbook
hfust	18.40 ± 0.50	kJ/mol	312.70	NIST Webbook
hsubt	109.10	kJ/mol	297.00	NIST Webbook
hvapt	69.90	kJ/mol	505.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	446.20	K	1.60	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters:	https://www.doi.org/10.1016/j.tca.2012.03.028
Investigation of the melting behavior of the reference materials biphenyl and phenyl salicylate by a new type adiabatic scanning calorimeter:	https://www.doi.org/10.1016/j.tca.2014.02.023
Solubility of Solol in Pure Alcohols from (283.15 to 308.15) K:	https://www.doi.org/10.1021/je800668j
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1154.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C118558&Units=SI
Thermodynamic Study of Phenyl Salicylate Solutions in Aprotic Solvents at Different Temperatures:	https://www.doi.org/10.1021/je8003595
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
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
hfust:	Enthalpy of fusion at a given temperature

hsubt:	Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume