O-(SALICYLOYLOXY)BENZOIC ACID

Other names:	2-Carboxyphenyl salicylate
	o-Salicylsalicylic acid
	Benzoic acid, 2-hydroxy-, 2-carboxyphenyl ester
	Diacesal
	Diplosal
	Disalcid
	Disalicylic acid
	Disalyl
	Nobacid
	Sal Ester Sal
	Salical
	Salicylic acid, bimolecular ester
	Salicylic acid, salicylate
	Salicyloylsalicylic acid
	Salicylsalicylic acid
	Salina
	Saloxium
	Salysal
	Sasapirin
	Sasapyrine
	Sasapyrinum
	NSC-49171
	SAA
	Sasapyrin
	2-Hydroxybenzoic acid 2-carboxyphenyl ester
	Disalgesic
	Mono-gesic
	Salflex
	Salicyl salicylate
	Salicyloxysalicylic acid
Inchi:	InChI=1S/C14H10O5/c15-11-7-3-1-5-9(11)14(18)19-12-8-4-2-6-10(12)13(16)17/h1-8,15H
InchiKey:	WVYADZUPLLSGPU-UHFFFAOYSA-N
Formula:	C14H10O5
SMILES:	O=C(Oc1ccccc1C(=O)O)c1ccccc1O
Mol. weight [g/mol]:	258.23

Physical Properties

Property code	Value	Unit	Source
chs	-5890.20	kJ/mol	NIST Webbook
hf	-681.64	kJ/mol	Cheméo Relay (1.0)
hfus	33.97	kJ/mol	Joback Method
hvap	124.60	kJ/mol	Cheméo Relay (1.0)
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-3.00		Cheméo Relay (1.0)
logp	2.310		Crippen Method
mcvol	181.350	ml/mol	McGowan Method
tb	616.34	K	Cheméo Relay (1.0)
tc	972.61	K	Cheméo Relay (1.0)
tf	409.73	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.98	J/mol×K	1078.17	Joback Method
cpg	561.15	J/mol×K	1117.60	Joback Method
cpg	522.57	J/mol×K	920.45	Joback Method
cpg	531.02	J/mol×K	959.88	Joback Method
cpg	539.00	J/mol×K	999.31	Joback Method
cpg	546.63	J/mol×K	1038.74	Joback Method
cpg	513.57	J/mol×K	881.02	Joback Method
dvisc	0.0000076	Pa×s	698.69	Joback Method
dvisc	0.0000146	Pa×s	653.11	Joback Method
dvisc	0.0000308	Pa×s	607.53	Joback Method
dvisc	0.0000043	Pa×s	744.28	Joback Method
dvisc	0.0000026	Pa×s	789.86	Joback Method
dvisc	0.0000017	Pa×s	835.44	Joback Method
dvisc	0.0000011	Pa×s	881.02	Joback Method
hfust	29.00	kJ/mol	430.20	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C552943&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point