Salicylic acid, n-octyl ester

Other names:	Benzoic acid, 2-hydroxy-, octyl ester
	Salicylic acid, octyl ester
	octyl salicylate
Inchi:	InChI=1S/C15H22O3/c1-2-3-4-5-6-9-12-18-15(17)13-10-7-8-11-14(13)16/h7-8,10-11,16H
InchiKey:	WCJLCOAEJIHPCW-UHFFFAOYSA-N
Formula:	C15H22O3
SMILES:	CCCCCCCCOC(=O)c1ccccc1O
Mol. weight [g/mol]:	250.33
CAS:	6969-49-9

Physical Properties

Property code	Value	Unit	Source
gf	-200.71	kJ/mol	Joback Method
hf	-538.51	kJ/mol	Joback Method
hfus	37.22	kJ/mol	Joback Method
hvap	73.43	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.910		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	1895.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1895.00		NIST Webbook
ripol	2435.00		NIST Webbook
tb	726.19	K	Joback Method
tc	932.89	K	Joback Method
tf	469.11	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.97	J/mol×K	726.19	Joback Method

cpg	619.96	J/mol×K	760.64	Joback Method
cpg	634.13	J/mol×K	795.09	Joback Method
cpg	647.52	J/mol×K	829.54	Joback Method
cpg	660.20	J/mol×K	863.99	Joback Method
cpg	672.24	J/mol×K	898.44	Joback Method
cpg	683.70	J/mol×K	932.89	Joback Method
dvisc	0.0003563	Pa×s	469.11	Joback Method
dvisc	0.0001558	Pa×s	511.96	Joback Method
dvisc	0.0000774	Pa×s	554.80	Joback Method
dvisc	0.0000425	Pa×s	597.65	Joback Method
dvisc	0.0000253	Pa×s	640.50	Joback Method
dvisc	0.0000161	Pa×s	683.34	Joback Method
dvisc	0.0000108	Pa×s	726.19	Joback Method

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6969499&Units=SI

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

ripol: Polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume