2-ETHYLHEXYL SALICYLATE

Other names:	Benzoic acid, 2-hydroxy-, 2-ethylhexyl ester
	Salicylic acid, 2-ethylhexyl ester
	Sunarome O
	Sunarome WMO
	USAF DO-11
	WMO
	Dermoblock OS
	Escalol 587
	Ethylhexyl salicylate
	Neo Heliopan OS
	Octyl salicylate
	Uvinul O-18
	2-Ethylhexyl 2-hydroxybenzoate
	NSC 46151
	Octisalate
Inchi:	InChI=1S/C15H22O3/c1-3-5-8-12(4-2)11-18-15(17)13-9-6-7-10-14(13)16/h6-7,9-10,12,1
InchiKey:	FMRHJJZUHUTGKE-UHFFFAOYSA-N
Formula:	C15H22O3
SMILES:	CCCCC(CC)COC(=O)c1ccccc1O
Mol. weight [g/mol]:	250.34

Physical Properties

Property code	Value	Unit	Source
hf	-614.77	kJ/mol	Cheméo Relay (1.0)
hfus	33.69	kJ/mol	Joback Method
hvap	82.62	kJ/mol	Cheméo Relay (1.0)
ie	8.35	eV	Cheméo Relay (1.0)
log10ws	-4.67		Cheméo Relay (1.0)
logp	3.765		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	1769.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1814.00		NIST Webbook
rinpol	1807.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1816.70		NIST Webbook

rinpol	1805.00		NIST Webbook
rinpol	1816.70		NIST Webbook
tb	584.29	K	Cheméo Relay (1.0)
tc	805.83	K	Cheméo Relay (1.0)
tf	237.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.51	J/mol×K	725.75	Joback Method
cpg	620.77	J/mol×K	760.76	Joback Method
cpg	635.15	J/mol×K	795.78	Joback Method
cpg	648.73	J/mol×K	830.79	Joback Method
cpg	661.57	J/mol×K	865.80	Joback Method
cpg	673.73	J/mol×K	900.82	Joback Method
cpg	685.30	J/mol×K	935.83	Joback Method
dvisc	0.0004694	Pa×s	454.11	Joback Method
dvisc	0.0001846	Pa×s	499.38	Joback Method
dvisc	0.0000848	Pa×s	544.66	Joback Method
dvisc	0.0000439	Pa×s	589.93	Joback Method
dvisc	0.0000249	Pa×s	635.20	Joback Method
dvisc	0.0000153	Pa×s	680.48	Joback Method
dvisc	0.0000100	Pa×s	725.75	Joback Method

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C118605&Units=SI

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

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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point