cis-3-Hexenyl salicylate

Other names:	Benzoic acid, 2-hydroxy-, 3-hexenyl ester, (Z)-
	Salicylic acid, 3-hexen-1-yl ester
	«beta»,«gamma»-cis-Hexenyl salicylate
	Salicylic acid, 3-hexenyl ester, (Z)-
	(3Z)-3-Hexenyl salicylate
	(Z)-3-Hexenyl salicylate
Inchi:	InChI=1S/C13H16O3/c1-2-3-4-7-10-16-13(15)11-8-5-6-9-12(11)14/h3-6,8-9,14H,2,7,10H
InchiKey:	IEPWIPZLLIOZLU-ARJAWSKDSA-N
Formula:	C13H16O3
SMILES:	CCC=CCCOC(=O)c1ccccc1O
Mol. weight [g/mol]:	220.26
CAS:	65405-77-8

Physical Properties

Property code	Value	Unit	Source
gf	-137.33	kJ/mol	Joback Method
hf	-380.01	kJ/mol	Joback Method
hfus	32.24	kJ/mol	Joback Method
hvap	68.94	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.905		Crippen Method
mcvol	179.280	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
rinpol	1640.80		NIST Webbook
rinpol	1643.70		NIST Webbook
rinpol	1629.10		NIST Webbook
rinpol	1644.30		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1647.80		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1654.55		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1640.80		NIST Webbook
rinpol	1651.80		NIST Webbook
rinpol	1636.10		NIST Webbook
rinpol	1637.70		NIST Webbook

rinpol	1649.40		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1643.70		NIST Webbook
rinpol	1643.70		NIST Webbook
ripol	2285.00		NIST Webbook
ripol	2274.00		NIST Webbook
ripol	2274.00		NIST Webbook
tb	684.59	K	Joback Method
tc	905.02	K	Joback Method
tf	441.49	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.20	J/mol×K	684.59	Joback Method
cpg	536.06	J/mol×K	868.28	Joback Method
cpg	525.40	J/mol×K	831.54	Joback Method
cpg	514.17	J/mol×K	794.80	Joback Method
cpg	502.29	J/mol×K	758.07	Joback Method
cpg	489.66	J/mol×K	721.33	Joback Method
cpg	546.22	J/mol×K	905.02	Joback Method
dvisc	0.0000140	Pa×s	684.59	Joback Method
dvisc	0.0000210	Pa×s	644.07	Joback Method
dvisc	0.0000333	Pa×s	603.56	Joback Method
dvisc	0.0000565	Pa×s	563.04	Joback Method
dvisc	0.0001039	Pa×s	522.52	Joback Method
dvisc	0.0002117	Pa×s	482.01	Joback Method
dvisc	0.0004917	Pa×s	441.49	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C65405778&Units=SI

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

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