(E)-Hex-3-enyl 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-ONEGZZNKSA-N
Formula: C13H16O3
SMILES: CCC=CCCOC(=O)c1ccccc1O
Mol. weight [g/mol]: 220.26

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	1648.00		NIST Webbook
rinpol	1648.00		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	489.66	J/mol×K	721.33	Joback Method
cpg	502.29	J/mol×K	758.07	Joback Method
cpg	514.17	J/mol×K	794.80	Joback Method
cpg	525.40	J/mol×K	831.54	Joback Method
cpg	536.06	J/mol×K	868.28	Joback Method
cpg	546.22	J/mol×K	905.02	Joback Method
dvisc	0.0004917	Pa×s	441.49	Joback Method

dvisc	0.0002117	Pa×s	482.01	Joback Method
dvisc	0.0001039	Pa×s	522.52	Joback Method
dvisc	0.0000565	Pa×s	563.04	Joback Method
dvisc	0.0000333	Pa×s	603.56	Joback Method
dvisc	0.0000210	Pa×s	644.07	Joback Method
dvisc	0.0000140	Pa×s	684.59	Joback Method

Sources

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=R292854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume