Benzoic acid, 2-hydroxy-, heptyl ester

Other names:	n-Heptyl salicylate
	heptyl salicylate
	heptyl 2-hydroxybenzoate
Inchi:	InChI=1S/C14H20O3/c1-2-3-4-5-8-11-17-14(16)12-9-6-7-10-13(12)15/h6-7,9-10,15H,2-5
InchiKey:	UGHVXXDQKXLCID-UHFFFAOYSA-N
Formula:	C14H20O3
SMILES:	CCCCCCCOC(=O)c1ccccc1O
Mol. weight [g/mol]:	236.31
CAS:	6259-77-4

Physical Properties

Property code	Value	Unit	Source
gf	-209.13	kJ/mol	Joback Method
hf	-517.87	kJ/mol	Joback Method
hfus	34.63	kJ/mol	Joback Method
hvap	71.20	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.519		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1785.00		NIST Webbook
rinpol	1789.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1790.00		NIST Webbook
ripol	2332.00		NIST Webbook
ripol	2332.00		NIST Webbook
tb	703.31	K	Joback Method
tc	912.60	K	Joback Method
tf	457.84	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.38	J/mol×K	703.31	Joback Method
cpg	616.46	J/mol×K	877.72	Joback Method
cpg	604.85	J/mol×K	842.84	Joback Method
cpg	592.60	J/mol×K	807.95	Joback Method
cpg	579.65	J/mol×K	773.07	Joback Method
cpg	565.93	J/mol×K	738.19	Joback Method
cpg	627.49	J/mol×K	912.60	Joback Method
dvisc	0.0000133	Pa×s	703.31	Joback Method
dvisc	0.0000199	Pa×s	662.40	Joback Method
dvisc	0.0000312	Pa×s	621.49	Joback Method
dvisc	0.0000523	Pa×s	580.58	Joback Method
dvisc	0.0000946	Pa×s	539.66	Joback Method
dvisc	0.0001888	Pa×s	498.75	Joback Method
dvisc	0.0004261	Pa×s	457.84	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6259774&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