Salicylic acid, p-octylphenyl ester

Inchi: InChI=1S/C21H26O3/c1-2-3-4-5-6-7-10-17-13-15-18(16-14-17)24-21(23)19-11-8-9-12-20
InchiKey: VNFXPOAMRORRJJ-UHFFFAOYSA-N
Formula: C21H26O3
SMILES: CCCCCCCCc1ccc(OC(=O)c2ccccc2O)cc1
Mol. weight [g/mol]: 326.43
CAS: 2512-56-3

Physical Properties

Property code	Value	Unit	Source
gf	-47.41	kJ/mol	Joback Method
hf	-437.29	kJ/mol	Joback Method
hfus	46.41	kJ/mol	Joback Method
hvap	89.72	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.514		Crippen Method
mcvol	272.540	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
tb	895.13	K	Joback Method
tc	1120.71	K	Joback Method
tf	575.67	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.21	J/mol×K	895.13	Joback Method
cpg	866.79	J/mol×K	932.73	Joback Method
cpg	881.51	J/mol×K	970.32	Joback Method
cpg	895.47	J/mol×K	1007.92	Joback Method
cpg	908.78	J/mol×K	1045.52	Joback Method
cpg	921.54	J/mol×K	1083.11	Joback Method
cpg	933.86	J/mol×K	1120.71	Joback Method
dvisc	0.0000721	Pa×s	575.67	Joback Method
dvisc	0.0000336	Pa×s	628.91	Joback Method

dvisc	0.0000177	Pa×s	682.16	Joback Method
dvisc	0.0000102	Pa×s	735.40	Joback Method
dvisc	0.0000063	Pa×s	788.64	Joback Method
dvisc	0.0000042	Pa×s	841.89	Joback Method
dvisc	0.0000029	Pa×s	895.13	Joback Method

Sources

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=C2512563&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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