

4-Chlorophenyl salicylate

Inchi:	InChI=1S/C13H9ClO3/c14-9-5-7-10(8-6-9)17-13(16)11-3-1-2-4-12(11)15/h1-8,15H
InchiKey:	TUYYMOBSJNEIKN-UHFFFAOYSA-N
Formula:	C13H9ClO3
SMILES:	O=C(Oc1ccc(Cl)cc1)c1ccccc1O
Mol. weight [g/mol]:	248.66
CAS:	2944-58-3

Physical Properties

Property code	Value	Unit	Source
gf	-126.70	kJ/mol	Joback Method
hf	-287.91	kJ/mol	Joback Method
hfus	29.89	kJ/mol	Joback Method
hvap	76.30	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.265		Crippen Method
mcvol	172.060	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	749.52	K	Joback Method
tc	1007.84	K	Joback Method
tf	515.43	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.08	J/mol×K	749.52	Joback Method
cpg	444.29	J/mol×K	792.57	Joback Method
cpg	454.62	J/mol×K	835.63	Joback Method
cpg	464.20	J/mol×K	878.68	Joback Method
cpg	473.13	J/mol×K	921.73	Joback Method
cpg	481.55	J/mol×K	964.79	Joback Method
cpg	489.56	J/mol×K	1007.84	Joback Method
dvisc	0.0001862	Pa×s	515.43	Joback Method
dvisc	0.0000994	Pa×s	554.45	Joback Method

dvisc	0.0000576	Pa×s	593.46	Joback Method
dvisc	0.0000357	Pa×s	632.48	Joback Method
dvisc	0.0000234	Pa×s	671.49	Joback Method
dvisc	0.0000160	Pa×s	710.50	Joback Method
dvisc	0.0000115	Pa×s	749.52	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=C2944583&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

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