

3-Methoxyphenyl salicylate

Inchi:	InChI=1S/C14H12O4/c1-17-10-5-4-6-11(9-10)18-14(16)12-7-2-3-8-13(12)15/h2-9,15H,1H
InchiKey:	QKOXLEURWZTLAY-UHFFFAOYSA-N
Formula:	C14H12O4
SMILES:	COc1cccc(OC(=O)c2ccccc2O)c1
Mol. weight [g/mol]:	244.24
CAS:	87720-40-9

Physical Properties

Property code	Value	Unit	Source
gf	-211.35	kJ/mol	Joback Method
hf	-425.03	kJ/mol	Joback Method
hfus	29.47	kJ/mol	Joback Method
hvap	76.55	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.620		Crippen Method
mcvol	179.780	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	757.39	K	Joback Method
tc	1004.09	K	Joback Method
tf	519.01	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.47	J/molxK	757.39	Joback Method
cpg	500.11	J/molxK	798.51	Joback Method
cpg	511.81	J/molxK	839.62	Joback Method
cpg	522.65	J/molxK	880.74	Joback Method
cpg	532.70	J/molxK	921.86	Joback Method
cpg	542.06	J/molxK	962.97	Joback Method
cpg	550.79	J/molxK	1004.09	Joback Method
dvisc	0.0001402	Paxs	519.01	Joback Method
dvisc	0.0000742	Paxs	558.74	Joback Method

dvisc	0.0000427	Paxs	598.47	Joback Method
dvisc	0.0000263	Paxs	638.20	Joback Method
dvisc	0.0000172	Paxs	677.93	Joback Method
dvisc	0.0000118	Paxs	717.66	Joback Method
dvisc	0.0000084	Paxs	757.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C87720409&Units=SI

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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