N-Salicylidene-m-aminobenzoic acid

Inchi: InChI=1S/C14H11NO3/c16-13-7-2-1-4-11(13)9-15-12-6-3-5-10(8-12)14(17)18/h1-9,16H,
InchiKey: MKFCCDWJBYFGJA-OQLLNIDSSA-N
Formula: C14H11NO3
SMILES: O=C(O)c1cccc(N=Cc2ccccc2O)c1
Mol. weight [g/mol]: 241.24
CAS: 841-12-3

Physical Properties

Property code	Value	Unit	Source
hf	-230.60	kJ/mol	Joback Method
hvap	91.72	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.841		Crippen Method
mcvol	179.590	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
tb	881.41	K	Joback Method
tc	1126.39	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	33.11	kJ/mol	464.00	NIST Webbook
sfust	71.36	J/mol×K	464.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C841123&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature