

Salicyl-3,4,5,6-d4-aldehyde-d

Inchi:	InChI=1S/C7H6O2/c8-5-6-3-1-2-4-7(6)9/h1-5,9H/i1D,2D,3D,4D,5D
InchiKey:	SMQUZDBALVYZAC-RALIUCGRSA-N
Formula:	C7HD5O2
SMILES:	O=Cc1ccccc1O
Mol. weight [g/mol]:	127.15

Physical Properties

Property code	Value	Unit	Source
gf	-133.67	kJ/mol	Joback Method
hf	-214.17	kJ/mol	Joback Method
hfus	16.00	kJ/mol	Joback Method
hvap	53.19	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.205		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
pc	5602.57	kPa	Joback Method
tb	515.52	K	Joback Method
tc	749.54	K	Joback Method
tf	348.79	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.64	J/molxK	515.52	Joback Method
cpg	206.73	J/molxK	554.52	Joback Method
cpg	215.05	J/molxK	593.53	Joback Method
cpg	222.66	J/molxK	632.53	Joback Method
cpg	229.65	J/molxK	671.53	Joback Method
cpg	236.10	J/molxK	710.54	Joback Method
cpg	242.09	J/molxK	749.54	Joback Method
dvisc	0.0031017	Paxs	348.79	Joback Method
dvisc	0.0014153	Paxs	376.58	Joback Method
dvisc	0.0007194	Paxs	404.37	Joback Method

dvisc	0.0003989	Paxs	432.15	Joback Method
dvisc	0.0002375	Paxs	459.94	Joback Method
dvisc	0.0001500	Paxs	487.73	Joback Method
dvisc	0.0000996	Paxs	515.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6007275&Units=SI
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

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
hvac:	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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