2-CARBAMOYL-1,4-DIHYDROXYBENZENE

Other names: Salicylamide, 5-hydroxy-
2,5-Dihydroxy benzamide
Inchi: InChI=1S/C7H7NO3/c8-7(11)5-3-4(9)1-2-6(5)10/h1-3,9-10H,(H2,8,11)
InchiKey: FRXZIFVYTNMCHF-UHFFFAOYSA-N
Formula: C7H7NO3
SMILES: NC(=O)c1cc(O)ccc1O
Mol. weight [g/mol]: 153.14

Physical Properties

Property code	Value	Unit	Source
hf	-491.60	kJ/mol	Cheméo Relay (1.0)
hfus	26.29	kJ/mol	Joback Method
log10ws	-1.37		Cheméo Relay (1.0)
logp	0.197		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
tb	572.98	K	Cheméo Relay (1.0)
tf	462.57	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.95	J/mol×K	673.88	Joback Method
cpg	286.51	J/mol×K	716.70	Joback Method
cpg	293.56	J/mol×K	759.53	Joback Method
cpg	300.26	J/mol×K	802.35	Joback Method
cpg	306.81	J/mol×K	845.17	Joback Method
cpg	313.36	J/mol×K	888.00	Joback Method
cpg	320.08	J/mol×K	930.82	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52405739&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point