3,4,5-Trihydroxybenzamide

Other names: Benzamide, 3,4,5-trihydroxy-
Gallamide
Inchi: InChI=1S/C7H7NO4/c8-7(12)3-1-4(9)6(11)5(10)2-3/h1-2,9-11H,(H2,8,12)
InchiKey: RBQIPEJXQPQFJX-UHFFFAOYSA-N
Formula: C7H7NO4
SMILES: NC(=O)c1cc(O)c(O)c(O)c1
Mol. weight [g/mol]: 169.13
CAS: 618-73-5

Physical Properties

Property code	Value	Unit	Source
gf	-405.86	kJ/mol	Joback Method
hf	-562.00	kJ/mol	Joback Method
hfus	32.07	kJ/mol	Joback Method
hvap	89.88	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	-0.098		Crippen Method
mcvol	114.890	ml/mol	McGowan Method
pc	10161.94	kPa	Joback Method
tb	754.50	K	Joback Method
tc	1017.67	K	Joback Method
tf	663.42	K	Joback Method
vc	0.253	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.71	J/mol×K	754.50	Joback Method
cpg	318.49	J/mol×K	798.36	Joback Method
cpg	325.32	J/mol×K	842.22	Joback Method
cpg	332.45	J/mol×K	886.08	Joback Method
cpg	340.13	J/mol×K	929.95	Joback Method
cpg	348.63	J/mol×K	973.81	Joback Method
cpg	358.18	J/mol×K	1017.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C618735&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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