2,4-Dihydroxybenzamide

Inchi: InChI=1S/C7H7NO3/c8-7(11)5-2-1-4(9)3-6(5)10/h1-3,9-10H,(H2,8,11)
InchiKey: IIUJCQYKTGNRHH-UHFFFAOYSA-N
Formula: C7H7NO3
SMILES: NC(=O)c1ccc(O)cc1O
Mol. weight [g/mol]: 153.14
CAS: 3147-45-3

Physical Properties

Property code	Value	Unit	Source
gf	-251.24	kJ/mol	Joback Method
hf	-384.69	kJ/mol	Joback Method
hfus	26.29	kJ/mol	Joback Method
hvap	76.87	kJ/mol	Joback Method
log10ws	-0.74		Crippen Method
logp	0.197		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	7681.19	kPa	Joback Method
tb	673.88	K	Joback Method
tc	930.82	K	Joback Method
tf	551.70	K	Joback Method
vc	0.286	m3/kmol	Joback Method

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

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=C3147453&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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