3-hydroxy-benzamide

Inchi: InChI=1S/C7H7NO2/c8-7(10)5-2-1-3-6(9)4-5/h1-4,9H,(H2,8,10)
InchiKey: NGMMGKYJUWYIIG-UHFFFAOYSA-N
Formula: C7H7NO2
SMILES: NC(=O)c1cccc(O)c1
Mol. weight [g/mol]: 137.14

Physical Properties

Property code	Value	Unit	Source
gf	-96.62	kJ/mol	Joback Method
hf	-207.38	kJ/mol	Joback Method
hfus	28.80	kJ/mol	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
hvap	63.85	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	0.491		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	6009.25	kPa	Joback Method
tb	593.26	K	Joback Method
tc	841.84	K	Joback Method
tf	440.70	K	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.37	J/mol×K	593.26	Joback Method
cpg	251.48	J/mol×K	634.69	Joback Method
cpg	259.81	J/mol×K	676.12	Joback Method
cpg	267.46	J/mol×K	717.55	Joback Method
cpg	274.53	J/mol×K	758.98	Joback Method
cpg	281.13	J/mol×K	800.41	Joback Method

cpg	287.34	J/mol×K	841.84	Joback Method
psub	8.21e-05	kPa	379.15	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	3.30e-05	kPa	369.65	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	3.84e-05	kPa	371.65	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	4.83e-05	kPa	374.15	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	5.78e-05	kPa	376.15	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	7.06e-05	kPa	377.15	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	2.62e-05	kPa	367.65	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	8.29e-05	kPa	379.65	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	9.16e-05	kPa	380.15	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	1.01e-04	kPa	381.65	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study

psub	1.29e-04	kPa	383.15	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	1.31e-04	kPa	383.65	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	1.44e-04	kPa	385.15	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	1.69e-04	kPa	386.15	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	1.92e-04	kPa	388.15	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	2.52e-04	kPa	390.15	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	3.07e-04	kPa	392.65	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	3.57e-04	kPa	394.15	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
psub	4.27e-04	kPa	396.15	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study:	https://www.doi.org/10.1016/j.tca.2012.10.013
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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