N-(hydroxymethyl)benzamide

Inchi: InChI=1S/C8H9NO2/c10-6-9-8(11)7-4-2-1-3-5-7/h1-5,10H,6H2,(H,9,11)
InchiKey: UOUBPDZUBVJZOQ-UHFFFAOYSA-N
Formula: C8H9NO2
SMILES: O=C(NCO)c1ccccc1
Mol. weight [g/mol]: 151.16
CAS: 6282-02-6

Physical Properties

Property code	Value	Unit	Source
gf	-47.46	kJ/mol	Joback Method
hf	-183.26	kJ/mol	Joback Method
hfus	21.30	kJ/mol	Joback Method
hvap	65.54	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	0.366		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
tb	605.34	K	Joback Method
tc	811.80	K	Joback Method
tf	369.75	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.01	J/mol×K	605.34	Joback Method
cpg	289.70	J/mol×K	639.75	Joback Method
cpg	298.74	J/mol×K	674.16	Joback Method
cpg	307.16	J/mol×K	708.57	Joback Method
cpg	315.01	J/mol×K	742.98	Joback Method
cpg	322.30	J/mol×K	777.39	Joback Method
cpg	329.07	J/mol×K	811.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6282026&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