N-Hydroxymethyl-2-phenylacetamide

Other names: N-Hydroxymethylphenylacetamide
Inchi: InChI=1S/C9H11NO2/c11-7-10-9(12)6-8-4-2-1-3-5-8/h1-5,11H,6-7H2,(H,10,12)
InchiKey: XXBWKSWPAMJCSC-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: O=C(Cc1ccccc1)NCO
Mol. weight [g/mol]: 165.19
CAS: 6291-06-1

Physical Properties

Property code	Value	Unit	Source
gf	-39.04	kJ/mol	Joback Method
hf	-203.90	kJ/mol	Joback Method
hfus	23.89	kJ/mol	Joback Method
hvap	67.77	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	0.295		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	628.22	K	Joback Method
tc	831.64	K	Joback Method
tf	381.02	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.78	J/mol×K	628.22	Joback Method
cpg	337.24	J/mol×K	662.12	Joback Method
cpg	347.03	J/mol×K	696.03	Joback Method
cpg	356.18	J/mol×K	729.93	Joback Method
cpg	364.71	J/mol×K	763.83	Joback Method
cpg	372.66	J/mol×K	797.73	Joback Method
cpg	380.06	J/mol×K	831.64	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6291061&Units=SI

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

Latest version available from:
https://www.chemeo.com/cid/36-079-5/N-Hydroxymethyl-2-phenylacetamide.pdf
Generated by Cheméo on 2024-10-12 05:48:01.010851891 +0000 UTC m=+3292943.647821140.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.