3,4-Methylenedioxybenzhydrazide

Other names: 1,3-Benzodioxole-5-carbohydrazide
Inchi: InChI=1S/C8H8N2O3/c9-10-8(11)5-1-2-6-7(3-5)13-4-12-6/h1-3H,4,9H2,(H,10,11)
InchiKey: RAXBGBHBUFGWPG-UHFFFAOYSA-N
Formula: C8H8N2O3
SMILES: NNC(=O)c1ccc2c(c1)OCO2
Mol. weight [g/mol]: 180.16
CAS: 22026-39-7

Physical Properties

Property code	Value	Unit	Source
gf	32.77	kJ/mol	Joback Method
hf	-191.04	kJ/mol	Joback Method
hfus	34.66	kJ/mol	Joback Method
hvap	70.07	kJ/mol	Joback Method
log10ws	-0.60		Aqueous Solubility Prediction Method
logp	0.019		Crippen Method
mcvol	122.230	ml/mol	McGowan Method
pc	5051.40	kPa	Joback Method
tb	660.96	K	Joback Method
tc	904.67	K	Joback Method
tf	492.55	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.07	J/mol×K	660.96	Joback Method
cpg	328.96	J/mol×K	701.58	Joback Method
cpg	338.03	J/mol×K	742.20	Joback Method
cpg	346.37	J/mol×K	782.82	Joback Method
cpg	354.04	J/mol×K	823.44	Joback Method
cpg	361.12	J/mol×K	864.06	Joback Method
cpg	367.68	J/mol×K	904.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22026397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume