4-phenylsemicarbazide

Inchi: InChI=1S/C7H9N3O/c8-10-7(11)9-6-4-2-1-3-5-6/h1-5H,8H2,(H2,9,10,11)
InchiKey: MOCKWYUCPREFCZ-UHFFFAOYSA-N
Formula: C7H9N3O
SMILES: NNC(=O)Nc1ccccc1
Mol. weight [g/mol]: 151.17

Physical Properties

Property code	Value	Unit	Source
gf	236.78	kJ/mol	Joback Method
hf	76.87	kJ/mol	Joback Method
hfus	24.92	kJ/mol	Joback Method
hvap	63.71	kJ/mol	Joback Method
log10ws	-2.33		Aqueous Solubility Prediction Method
logp	0.682		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	5008.59	kPa	Joback Method
tb	612.98	K	Joback Method
tc	847.56	K	Joback Method
tf	433.58	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.95	J/mol×K	612.98	Joback Method
cpg	296.72	J/mol×K	652.08	Joback Method
cpg	306.66	J/mol×K	691.17	Joback Method
cpg	315.80	J/mol×K	730.27	Joback Method
cpg	324.19	J/mol×K	769.36	Joback Method
cpg	331.88	J/mol×K	808.46	Joback Method
cpg	338.89	J/mol×K	847.56	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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