

(R)-(-)-2-Phenylglycine

Other names:	D-(-)-«alpha»-Phenylglycine R(-)-«alpha»-Aminophenylacetic acid D(-)«alpha»-Aminophenylacetic acid D-(-)-Phenylglycine D-2-Phenylglycine Benzeneacetic acid, «alpha»-amino-, (R)- Amino(phenyl)acetic acid -, (alphaR)- d-«alpha»-Phenylglycine
Inchi:	InChI=1S/C8H9NO2/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5,7H,9H2,(H,10,11)/t7-/m0/s1
InchiKey:	ZGUNAGUHMKGQNY-ZETCQYMHSA-N
Formula:	C8H9NO2
SMILES:	NC(C(=O)O)c1ccccc1
Mol. weight [g/mol]:	151.16
CAS:	875-74-1

Physical Properties

Property code	Value	Unit	Source
gf	-72.84	kJ/mol	Joback Method
hf	-208.22	kJ/mol	Joback Method
hfus	17.88	kJ/mol	Joback Method
hsub	165.00 ± 6.00	kJ/mol	NIST Webbook
hvap	69.36	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	0.771		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4856.20	kPa	Joback Method
tb	627.26	K	Joback Method
tc	845.92	K	Joback Method
tf	385.35	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	329.16	J/mol×K	809.48	Joback Method
cpg	287.79	J/mol×K	627.26	Joback Method
cpg	297.38	J/mol×K	663.70	Joback Method
cpg	306.27	J/mol×K	700.15	Joback Method
cpg	314.51	J/mol×K	736.59	Joback Method
cpg	322.13	J/mol×K	773.03	Joback Method
cpg	335.63	J/mol×K	845.92	Joback Method
hsubt	148.90 ± 2.20	kJ/mol	443.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C875741&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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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

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