

(R)-(-)-2-PHENYLGLYCINOL

Other names:	(R)-«beta»-aminophenethyl alcohol Benzeneethanol, «beta»-amino-, (R)-
Inchi:	InChI=1S/C8H11NO/c9-8(6-10)7-4-2-1-3-5-7/h1-5,8,10H,6,9H2/t8-/m0/s1
InchiKey:	IJXJGQCXFSSHNL-MRVPVSSYSA-N
Formula:	C8H11NO
SMILES:	N[C@@H](CO)c1ccccc1
Mol. weight [g/mol]:	137.18

Physical Properties

Property code	Value	Unit	Source
hf	-109.77	kJ/mol	Cheméo Relay (1.0)
hfus	16.28	kJ/mol	Joback Method
hvap	72.75	kJ/mol	Cheméo Relay (1.0)
ie	8.72	eV	Cheméo Relay (1.0)
log10ws	-0.83		Cheméo Relay (1.0)
logp	0.679		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
tb	557.61	K	Cheméo Relay (1.0)
tf	349.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.53	J/mol×K	573.39	Joback Method
cpg	287.40	J/mol×K	608.62	Joback Method
cpg	297.57	J/mol×K	643.84	Joback Method
cpg	307.08	J/mol×K	679.07	Joback Method
cpg	315.94	J/mol×K	714.30	Joback Method
cpg	324.21	J/mol×K	749.52	Joback Method
cpg	331.92	J/mol×K	784.75	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C56613800&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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