Alanine, n-amino-3-phenyl-, dl-

Inchi: InChI=1S/C9H12N2O2/c10-11-8(9(12)13)6-7-4-2-1-3-5-7/h1-5,8,11H,6,10H2,(H,12,13)
InchiKey: KHZVLGLEHBZEPO-UHFFFAOYSA-N
Formula: C9H12N2O2
SMILES: NNC(Cc1ccccc1)C(=O)O
Mol. weight [g/mol]: 180.20
CAS: 1421-34-7

Physical Properties

Property code	Value	Unit	Source
gf	24.97	kJ/mol	Joback Method
hf	-175.39	kJ/mol	Joback Method
hfus	25.57	kJ/mol	Joback Method
hvap	78.02	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	0.146		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	700.31	K	Joback Method
tc	914.56	K	Joback Method
tf	449.28	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.27	J/mol×K	700.31	Joback Method
cpg	391.41	J/mol×K	736.02	Joback Method
cpg	400.82	J/mol×K	771.73	Joback Method
cpg	409.53	J/mol×K	807.44	Joback Method
cpg	417.59	J/mol×K	843.15	Joback Method
cpg	425.03	J/mol×K	878.86	Joback Method
cpg	431.90	J/mol×K	914.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1421347&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
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