2-Azetidinone, 4-phenyl-

Other names: Benzenepropanoic acid, «beta»-amino-, lactam
4-Phenyl-2-azetidinone
Inchi: InChI=1S/C9H9NO/c11-9-6-8(10-9)7-4-2-1-3-5-7/h1-5,8H,6H2,(H,10,11)
InchiKey: MWKMQPSNTJCASD-UHFFFAOYSA-N
Formula: C9H9NO
SMILES: OC1=NC(c2ccccc2)C1
Mol. weight [g/mol]: 147.17
CAS: 5661-55-2

Physical Properties

Property code	Value	Unit	Source
gf	186.25	kJ/mol	Joback Method
hf	39.13	kJ/mol	Joback Method
hfus	19.20	kJ/mol	Joback Method
hvap	61.83	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.088		Crippen Method
mcvol	114.600	ml/mol	McGowan Method
pc	4553.06	kPa	Joback Method
rinpol	1254.00		NIST Webbook
rinpol	1254.00		NIST Webbook
tb	593.03	K	Joback Method
tc	821.51	K	Joback Method
tf	377.67	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.26	J/mol×K	593.03	Joback Method
cpg	303.14	J/mol×K	631.11	Joback Method
cpg	315.09	J/mol×K	669.19	Joback Method
cpg	326.14	J/mol×K	707.27	Joback Method
cpg	336.35	J/mol×K	745.35	Joback Method

cpg	345.74	J/mol×K	783.43	Joback Method
cpg	354.36	J/mol×K	821.51	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5661552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume