Hexanoic acid, 6-(carboxyamino)-, n-benzyl ester

Other names: 6-[[(phenylmethoxy)carbonyl]amino]hexanoic acid
Inchi: InChI=1S/C14H19NO4/c16-13(17)9-5-2-6-10-15-14(18)19-11-12-7-3-1-4-8-12/h1,3-4,7-8
InchiKey: RXQDBVWDABAAHL-UHFFFAOYSA-N
Formula: C14H19NO4
SMILES: O=C(O)CCCCCNC(=O)OCc1ccccc1
Mol. weight [g/mol]: 265.31
CAS: 1947-00-8

Physical Properties

Property code	Value	Unit	Source
gf	-230.86	kJ/mol	Joback Method
hf	-551.90	kJ/mol	Joback Method
hfus	39.63	kJ/mol	Joback Method
hvap	88.05	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.558		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
tb	818.91	K	Joback Method
tc	1019.78	K	Joback Method
tf	509.53	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.14	J/mol×K	818.91	Joback Method
cpg	633.71	J/mol×K	852.39	Joback Method
cpg	644.45	J/mol×K	885.87	Joback Method
cpg	654.38	J/mol×K	919.35	Joback Method
cpg	663.53	J/mol×K	952.83	Joback Method
cpg	671.94	J/mol×K	986.30	Joback Method
cpg	679.64	J/mol×K	1019.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1947008&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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