Hexanoic acid, 6-(benzoylamino)-

Other names: Hexanoic acid, «epsilon»-benzamido-
6-Benzamidohexanoic acid
E-Benzamido coproic acid
Inchi: InChI=1S/C13H17NO3/c15-12(16)9-5-2-6-10-14-13(17)11-7-3-1-4-8-11/h1,3-4,7-8H,2,5-
InchiKey: LFCIOBCYMAQQBT-UHFFFAOYSA-N
Formula: C13H17NO3
SMILES: O=C(O)CCCCCNC(=O)c1ccccc1
Mol. weight [g/mol]: 235.28
CAS: 956-09-2

Physical Properties

Property code	Value	Unit	Source
gf	-134.28	kJ/mol	Joback Method
hf	-399.04	kJ/mol	Joback Method
hfus	35.85	kJ/mol	Joback Method
hvap	83.41	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.061		Crippen Method
mcvol	189.260	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	773.61	K	Joback Method
tc	975.10	K	Joback Method
tf	476.03	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.91	J/mol×K	773.61	Joback Method
cpg	553.32	J/mol×K	807.19	Joback Method
cpg	563.95	J/mol×K	840.77	Joback Method
cpg	573.86	J/mol×K	874.35	Joback Method
cpg	583.07	J/mol×K	907.94	Joback Method
cpg	591.63	J/mol×K	941.52	Joback Method

cpg	599.57	J/mol×K	975.10	Joback Method

Sources

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=C956092&Units=SI
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
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