

8-Aminocaprylic acid

Other names:	«omega»-Aminocaprylic acid Octanoic acid, 8-amino- 8-aminooctanoic acid
Inchi:	InChI=1S/C8H17NO2/c9-7-5-3-1-2-4-6-8(10)11/h1-7,9H2,(H,10,11)
InchiKey:	UQXNEWQGGVUVQA-UHFFFAOYSA-N
Formula:	C8H17NO2
SMILES:	NCCCCCCCC(=O)O
Mol. weight [g/mol]:	159.23
CAS:	1002-57-9

Physical Properties

Property code	Value	Unit	Source
chs	-4884.00	kJ/mol	NIST Webbook
gf	-182.81	kJ/mol	Joback Method
hf	-524.00 ± 4.00	kJ/mol	NIST Webbook
hfs	-694.00	kJ/mol	NIST Webbook
hfus	27.36	kJ/mol	Joback Method
hsub	170.00 ± 4.00	kJ/mol	NIST Webbook
hsub	170.00 ± 4.00	kJ/mol	NIST Webbook
hvap	67.47	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.370		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	601.02	K	Joback Method
tc	779.44	K	Joback Method
tf	373.93	K	Joback Method
vc	0.537	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.90	J/mol×K	601.02	Joback Method
cpg	377.79	J/mol×K	630.76	Joback Method

cpg	388.17	J/mol×K	660.49	Joback Method
cpg	398.06	J/mol×K	690.23	Joback Method
cpg	407.48	J/mol×K	719.96	Joback Method
cpg	416.44	J/mol×K	749.70	Joback Method
cpg	424.95	J/mol×K	779.44	Joback Method
cps	251.70	J/mol×K	298.00	NIST Webbook
hsubt	166.20 ± 0.90	kJ/mol	396.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1002579&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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

Latest version available from:

<https://www.cheméo.com/cid/23-736-9/8-Aminocaprylic-acid.pdf>

Generated by Cheméo on 2024-04-28 18:44:04.557472101 +0000 UTC m=+16619093.478049417.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.