

OCTANOIC ACID, 2-AMINO-

Other names:	dl-«alpha»-Amino-n-caprylic acid dl-2-Aminooctanoic acid Octanoic acid, 2-amino-, (.+/-.)- Octanoic acid, 2-amino-, DL- 2-Amino-DL-caprylic acid 2-Aminooctanoic acid Octanoic acid, 2-amino- NSC 20147 «alpha»-Aminocaprylic acid (±)-2-aminooctanoic acid
Inchi:	InChI=1S/C8H17NO2/c1-2-3-4-5-6-7(9)8(10)11/h7H,2-6,9H2,1H3,(H,10,11)
InchiKey:	AKVBCGQVQXPRLD-UHFFFAOYSA-N
Formula:	C8H17NO2
SMILES:	CCCCCCC(N)C(=O)O
Mol. weight [g/mol]:	159.23

Physical Properties

Property code	Value	Unit	Source
af	0.7759		Cheméo Relay (1.0)
gf	-185.25	kJ/mol	Joback Method
hf	-532.26	kJ/mol	Cheméo Relay (1.0)
hfus	23.84	kJ/mol	Joback Method
hvap	78.25	kJ/mol	Cheméo Relay (1.0)
ie	8.83	eV	Cheméo Relay (1.0)
log10ws	-1.89		Cheméo Relay (1.0)
logp	1.369		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
tb	532.26	K	Cheméo Relay (1.0)
tc	708.61	K	Cheméo Relay (1.0)
tf	447.20	K	Cheméo Relay (1.0)
vc	0.507	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.35	J/mol×K	600.58	Joback Method
cpg	378.47	J/mol×K	630.83	Joback Method
cpg	389.06	J/mol×K	661.08	Joback Method
cpg	399.14	J/mol×K	691.33	Joback Method
cpg	408.71	J/mol×K	721.58	Joback Method
cpg	417.81	J/mol×K	751.83	Joback Method
cpg	426.44	J/mol×K	782.09	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C644906&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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