2-AMINO-4-PENTENOIC ACID

Other names:	dl-2-Amino-1-pentenoic acid
	4-Pentenoic acid, 2-amino-, (.+/-.)-
	2-Amino-4-pentenoic acid
	DL-2-aminopent-4-enoic acid
Inchi:	InChI=1S/C5H9NO2/c1-2-3-4(6)5(7)8/h2,4H,1,3,6H2,(H,7,8)
InchiKey:	WNNNWFKQCKFSDK-UHFFFAOYSA-N
Formula:	C5H9NO2
SMILES:	C=CCC(N)C(=O)O
Mol. weight [g/mol]:	115.13

Physical Properties

Property code	Value	Unit	Source
hfus	14.79	kJ/mol	Joback Method
ie	8.93	eV	Cheméo Relay (1.0)
log10ws	-0.07		Cheméo Relay (1.0)
logp	-0.026		Crippen Method
mcvol	94.430	ml/mol	McGowan Method
tb	486.60	K	Cheméo Relay (1.0)
tf	419.95	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.68	J/mol×K	528.62	Joback Method
cpg	221.39	J/mol×K	560.44	Joback Method
cpg	228.69	J/mol×K	592.26	Joback Method
cpg	235.61	J/mol×K	624.08	Joback Method
cpg	242.15	J/mol×K	655.90	Joback Method
cpg	248.33	J/mol×K	687.72	Joback Method
cpg	254.16	J/mol×K	719.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7685441&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point