7-aminoheptanoic acid

Inchi: InChI=1S/C7H15NO2/c8-6-4-2-1-3-5-7(9)10/h1-6,8H2,(H,9,10)
InchiKey: XDOLZJYETYVRKV-UHFFFAOYSA-N
Formula: C7H15NO2
SMILES: NCCCCCCC(=O)O
Mol. weight [g/mol]: 145.20
CAS: 929-17-9

Physical Properties

Property code	Value	Unit	Source
chs	-4608.70	kJ/mol	NIST Webbook
chs	-4230.90 ± 1.30	kJ/mol	NIST Webbook
gf	-191.23	kJ/mol	Joback Method
hf	-418.83	kJ/mol	Joback Method
hfus	24.77	kJ/mol	Joback Method
hvap	65.24	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	0.980		Crippen Method
mcvol	126.910	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
tb	578.14	K	Joback Method
tc	758.06	K	Joback Method
tf	362.66	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.04	J/mol×K	578.14	Joback Method
cpg	330.13	J/mol×K	608.13	Joback Method
cpg	339.75	J/mol×K	638.11	Joback Method
cpg	348.92	J/mol×K	668.10	Joback Method
cpg	357.65	J/mol×K	698.09	Joback Method
cpg	365.95	J/mol×K	728.07	Joback Method
cpg	373.84	J/mol×K	758.06	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=C929179&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
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