D-glutamic acid

Inchi: InChI=1S/C5H9NO4/c6-3(5(9)10)1-2-4(7)8/h3H,1-2,6H2,(H,7,8)(H,9,10)/t3-/m0/s1
InchiKey: WHUUTDBJXJRKMK-VKHMYHEASA-N
Formula: C5H9NO4
SMILES: NC(CCC(=O)O)C(=O)O
Mol. weight [g/mol]: 147.13
CAS: 6893-26-1

Physical Properties

Property code	Value	Unit	Source
chs	-2251.32 ± 0.68	kJ/mol	NIST Webbook
chs	-2248.10 ± 1.20	kJ/mol	NIST Webbook
gf	-476.25	kJ/mol	Joback Method
hf	-647.64	kJ/mol	Joback Method
hfs	-1002.47 ± 0.07	kJ/mol	NIST Webbook
hfs	-1009.60	kJ/mol	NIST Webbook
hfus	21.75	kJ/mol	Joback Method
hvap	83.83	kJ/mol	Joback Method
log10ws	0.34		Crippen Method
logp	-0.737		Crippen Method
mcvol	106.170	ml/mol	McGowan Method
pc	5713.21	kPa	Joback Method
ss	191.20	J/mol×K	NIST Webbook
tb	677.99	K	Joback Method
tc	864.26	K	Joback Method
tf	435.87	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.71	J/mol×K	677.99	Joback Method
cpg	286.05	J/mol×K	709.03	Joback Method
cpg	292.03	J/mol×K	740.08	Joback Method
cpg	297.65	J/mol×K	771.12	Joback Method

cpg	302.93	J/mol×K	802.17	Joback Method
cpg	307.87	J/mol×K	833.21	Joback Method
cpg	312.49	J/mol×K	864.26	Joback Method
cps	172.80	J/mol×K	294.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6893261&Units=SI

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
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume