Ethylenediamine-N,N'-disuccinic acid

Inchi: InChI=1S/C10H16N2O8/c13-7(14)3-5(9(17)18)11-1-2-12-6(10(19)20)4-8(15)16/h5-6,11-1
InchiKey: VKZRWSNIWNFCIQ-UHFFFAOYSA-N
Formula: C10H16N2O8
SMILES: O=C(O)CC(NCCNC(CC(=O)O)C(=O)O)C(=O)O
Mol. weight [g/mol]: 292.24
CAS: 20846-91-7

Physical Properties

Property code	Value	Unit	Source
chs	-4271.60 ± 3.90	kJ/mol	NIST Webbook
chs	-4252.10 ± 4.20	kJ/mol	NIST Webbook
gf	-855.74	kJ/mol	Joback Method
hf	-1212.59	kJ/mol	Joback Method
hfs	-1969.40 ± 4.20	kJ/mol	NIST Webbook
hfs	-1950.20 ± 3.90	kJ/mol	NIST Webbook
hfus	47.56	kJ/mol	Joback Method
hvap	143.65	kJ/mol	Joback Method
log10ws	0.99		Crippen Method
logp	-1.979		Crippen Method
mcvol	201.480	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
tb	1111.86	K	Joback Method
tc	1391.50	K	Joback Method
tf	720.78	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.18	J/mol×K	1111.86	Joback Method
cpg	665.03	J/mol×K	1158.47	Joback Method
cpg	669.93	J/mol×K	1205.07	Joback Method
cpg	673.98	J/mol×K	1251.68	Joback Method
cpg	677.25	J/mol×K	1298.29	Joback Method

cpg	679.82	J/mol×K	1344.89	Joback Method
cpg	681.77	J/mol×K	1391.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20846917&Units=SI
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

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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