Succinimide

Other names:	2,5-Diketopyrrolidine
	2,5-Dioxopyrrolidine
	2,5-Pyrrolidinedione
	3,4-Dihydropyrrole-2,5-dione
	Butanimide
	Dihydro-3-pyrroline-2,5-dione
	Lubrizol 6406
	NSC 11204
	Succinic acid imide
	Succinic imide
	Succinimide-Sauba
Inchi:	InChI=1S/C4H5NO2/c6-3-1-2-4(7)5-3/h1-2H2,(H,5,6,7)
InchiKey:	KZNICNPSHKQLFF-UHFFFAOYSA-N
Formula:	C4H5NO2
SMILES:	O=C1CCC(=O)N1
Mol. weight [g/mol]:	99.09
CAS:	123-56-8

Physical Properties

Property code	Value	Unit	Source
chs	-1829.60 ± 0.20	kJ/mol	NIST Webbook
chs	-1828.36 ± 0.24	kJ/mol	NIST Webbook
gf	-130.41	kJ/mol	Joback Method
hf	-362.20 ± 9.30	kJ/mol	NIST Webbook
hf	-375.50 ± 1.50	kJ/mol	NIST Webbook
hfs	-460.25 ± 0.30	kJ/mol	NIST Webbook
hfs	-459.10 ± 0.30	kJ/mol	NIST Webbook
hfus	7.59	kJ/mol	Joback Method
hsub	98.10 ± 4.50	kJ/mol	NIST Webbook
hsub	83.60 ± 1.50	kJ/mol	NIST Webbook
hsub	83.60 ± 1.50	kJ/mol	NIST Webbook
hvap	40.32	kJ/mol	Joback Method
ie	10.01	eV	NIST Webbook
ie	10.01	eV	NIST Webbook
log10ws	0.30		Estimated Solubility Method

log10ws	0.30		Aqueous Solubility Prediction Method
logp	-0.577		Crippen Method
mcvol	69.480	ml/mol	McGowan Method
pc	5972.16	kPa	Joback Method
ripol	2458.00		NIST Webbook
ripol	2458.00		NIST Webbook
tb	560.70	K	NIST Webbook
tc	747.16	K	Joback Method
tf	400.00 ± 1.50	K	NIST Webbook
tf	398.40	K	Aqueous Solubility Prediction Method
tf	398.15 ± 0.60	K	NIST Webbook
vc	0.253	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.41	J/mol×K	579.09	Joback Method
cpg	151.36	J/mol×K	537.08	Joback Method
cpg	197.52	J/mol×K	747.16	Joback Method
cpg	189.24	J/mol×K	705.14	Joback Method
cpg	180.42	J/mol×K	663.12	Joback Method
cpg	171.12	J/mol×K	621.11	Joback Method
cpg	141.03	J/mol×K	495.06	Joback Method
cps	123.88	J/mol×K	298.15	NIST Webbook
cps	131.40	J/mol×K	323.00	NIST Webbook
hfust	17.00	kJ/mol	400.00	NIST Webbook
hfust	17.00	kJ/mol	400.00	NIST Webbook
hfust	17.00	kJ/mol	400.00	NIST Webbook
hsubt	83.10 ± 1.50	kJ/mol	328.50	NIST Webbook
hvapt	73.50	kJ/mol	474.00	NIST Webbook
hvapt	66.90	kJ/mol	488.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C123568&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solubilities of succinimide in different pure solvents and binary methanol+ethyl acetate solvent mixtures:	https://www.doi.org/10.1016/j.tca.2012.03.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume