N-Methylsuccinimide

Other names: Succinimide, N-methyl-
N-Methylsuccinimide
1-Methyl-2,5-pyrrolidinedione
Inchi: InChI=1S/C5H7NO2/c1-6-4(7)2-3-5(6)8/h2-3H2,1H3
InchiKey: KYEACNNYFNZCST-UHFFFAOYSA-N
Formula: C5H7NO2
SMILES: CN1C(=O)CCC1=O
Mol. weight [g/mol]: 113.12

Physical Properties

Property code	Value	Unit	Source
chs	-2498.10 ± 1.50	kJ/mol	NIST Webbook
hf	-389.70 ± 1.60	kJ/mol	NIST Webbook
hfs	-469.80 ± 1.60	kJ/mol	NIST Webbook
hsub	80.10 ± 0.30	kJ/mol	NIST Webbook
hsub	80.10 ± 0.30	kJ/mol	NIST Webbook
hvap	54.90	kJ/mol	Cheméo Relay (1.0)
ie	10.71	eV	NIST Webbook
log10ws	0.38		Cheméo Relay (1.0)
logp	-0.235		Crippen Method
mcvol	83.570	ml/mol	McGowan Method
pc	4672.70	kPa	Cheméo Relay (1.0, beta)
ripol	1910.00		NIST Webbook
ripol	1910.00		NIST Webbook
tb	507.20	K	NIST Webbook
tc	729.50	K	Cheméo Relay (1.0)
tf	399.86	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	80.60 ± 0.30	kJ/mol	289.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.50 ± 1.50	K	2.70	NIST Webbook

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121079&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point