MALONAMIDE

Other names:	1,3-propanedioic acid, diamide
	Carboxamidoacetamide
	Malondiamide
	Malonyldiamide
	malonic acid diamide
	malonodiamide
Inchi:	InChI=1S/C3H6N2O2/c4-2(6)1-3(5)7/h1H2,(H2,4,6)(H2,5,7)
InchiKey:	WRIRWRKPLXCTFD-UHFFFAOYSA-N
Formula:	C3H6N2O2
SMILES:	NC(=O)CC(N)=O
Mol. weight [g/mol]:	102.09

Physical Properties

Property code	Value	Unit	Source
chs	-1491.90 ± 1.50	kJ/mol	NIST Webbook
chs	-1495.21 ± 0.26	kJ/mol	NIST Webbook
hf	-416.40 ± 0.40	kJ/mol	NIST Webbook
hfs	-546.10 ± 1.50	kJ/mol	NIST Webbook
hfs	-542.81 ± 0.53	kJ/mol	NIST Webbook
hfus	29.85	kJ/mol	Odd even effect in melting properties of 12 alkane-a,x-diamides
hfus	23.22	kJ/mol	Reconciling thermal and structural data from the polymorphic transitions of malonamide
hsub	126.40 ± 0.50	kJ/mol	NIST Webbook
hvap	57.68	kJ/mol	Cheméo Relay (1.0)
ie	9.85	eV	Cheméo Relay (1.0)
log10ws	-0.42		Cheméo Relay (1.0)
logp	-1.653		Crippen Method
mcvol	76.230	ml/mol	McGowan Method
rinpol	1125.00		NIST Webbook
tb	483.53	K	Cheméo Relay (1.0)
tf	426.02	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.41	J/mol×K	705.19	Joback Method
cpg	184.91	J/mol×K	631.45	Joback Method
cpg	200.13	J/mol×K	742.06	Joback Method
cpg	190.34	J/mol×K	668.32	Joback Method
cpg	166.39	J/mol×K	520.84	Joback Method
cpg	172.95	J/mol×K	557.71	Joback Method
cpg	179.12	J/mol×K	594.58	Joback Method
cps	124.00	J/mol×K	298.15	NIST Webbook
hfust	29.85	kJ/mol	444.20	NIST Webbook
hfust	35.80	kJ/mol	443.00	NIST Webbook
hfust	1.90	kJ/mol	393.00	NIST Webbook
hfust	35.80	kJ/mol	443.00	NIST Webbook
hsubt	126.40	kJ/mol	298.15	NIST Webbook
sfust	4.83	J/mol×K	393.00	NIST Webbook
sfust	80.81	J/mol×K	443.00	NIST Webbook
ssubt	423.90	J/mol×K	298.15	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Odd even effect in melting properties of 12 alkane-a,x-diamides: https://www.doi.org/10.1016/j.jct.2006.04.004

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C108134&Units=SI

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

Reconciling thermal and structural data from the polymorphic transitions of malonamide: https://www.doi.org/10.1016/j.tca.2008.10.019

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

cps:	Solid phase heat capacity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ssubt:	Entropy of sublimation at a given temperature
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point