

2-METHYLMALONODIAMIDE

Other names:	2-Methylmalonamide
Inchi:	InChI=1S/C4H8N2O2/c1-2(3(5)7)4(6)8/h2H,1H3,(H2,5,7)(H2,6,8)
InchiKey:	CGRKYGKHZOCPSZ-UHFFFAOYSA-N
Formula:	C4H8N2O2
SMILES:	CC(C(N)=O)C(N)=O
Mol. weight [g/mol]:	116.12

Physical Properties

Property code	Value	Unit	Source
hf	-500.85	kJ/mol	Cheméo Relay (1.0)
hfus	16.18	kJ/mol	Joback Method
hvap	57.72	kJ/mol	Cheméo Relay (1.0)
ie	9.53	eV	Cheméo Relay (1.0)
log10ws	-0.35		Cheméo Relay (1.0)
logp	-1.407		Crippen Method
mcvol	90.320	ml/mol	McGowan Method
tb	480.41	K	Cheméo Relay (1.0)
tf	420.56	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.49	J/mol×K	543.28	Joback Method
cpg	215.58	J/mol×K	580.33	Joback Method
cpg	223.19	J/mol×K	617.39	Joback Method
cpg	230.32	J/mol×K	654.44	Joback Method
cpg	236.99	J/mol×K	691.49	Joback Method
cpg	243.21	J/mol×K	728.54	Joback Method
cpg	248.99	J/mol×K	765.60	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1113639&Units=SI>

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

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

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):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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