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
CAS: 1113-63-9

Physical Properties

Property code	Value	Unit	Source
gf	-144.58	kJ/mol	Joback Method
hf	-288.75	kJ/mol	Joback Method
hfus	16.18	kJ/mol	Joback Method
hvap	58.88	kJ/mol	Joback Method
log10ws	0.33		Crippen Method
logp	-1.407		Crippen Method
mcvol	90.320	ml/mol	McGowan Method
pc	5454.60	kPa	Joback Method
tb	543.28	K	Joback Method
tc	765.60	K	Joback Method
tf	386.22	K	Joback Method
vc	0.324	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1113639&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

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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