Malonanilic acid

Inchi: InChI=1S/C9H9NO3/c11-8(6-9(12)13)10-7-4-2-1-3-5-7/h1-5H,6H2,(H,10,11)(H,12,13)
InchiKey: NOJXRHBIVBIMQY-UHFFFAOYSA-N
Formula: C9H9NO3
SMILES: O=C(O)CC(=O)Nc1ccccc1
Mol. weight [g/mol]: 179.17
CAS: 15580-32-2

Physical Properties

Property code	Value	Unit	Source
gf	-167.96	kJ/mol	Joback Method
hf	-316.48	kJ/mol	Joback Method
hfus	25.49	kJ/mol	Joback Method
hvap	74.51	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.100		Crippen Method
mcvol	132.900	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method
tb	682.09	K	Joback Method
tc	892.20	K	Joback Method
tf	430.95	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.18	J/mol×K	682.09	Joback Method
cpg	346.36	J/mol×K	717.11	Joback Method
cpg	354.86	J/mol×K	752.13	Joback Method
cpg	362.73	J/mol×K	787.15	Joback Method
cpg	370.00	J/mol×K	822.16	Joback Method
cpg	376.69	J/mol×K	857.18	Joback Method
cpg	382.84	J/mol×K	892.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15580322&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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