Butanedioic acid, mono(2,2-dimethylhydrazide)

Other names: Alar
Alar 85
Aminozid
Aminozide
B 995
B-Nine
DMASA
DYaK
Daminozide
Dazide
Dimas
Dimethylaminosuccinamic acid
Kylar
N-(Dimethylamino)succinamic acid
SADH
Succinic N',N'-dimethylhydrazide
Succinic acid, 2,2-dimethylhydrazide
Succinic acid, N,N-dimethylhydrazide
Succinic acid, mono(2,2-dimethylhydrazide)
Succinic acid, mono-2,2-dimethylhydrazine

Inchi: InChI=1S/C6H12N2O3/c1-8(2)7-5(9)3-4-6(10)11/h3-4H2,1-2H3,(H,7,9)(H,10,11)

InchiKey: NOQGZXFMHARMLW-UHFFFAOYSA-N

Formula: C6H11NO3

SMILES: CN(C)NC(=O)CCC(=O)O

Mol. weight [g/mol]: 145.16

CAS: 1596-84-5

Physical Properties

Property code	Value	Unit	Source
gf	-194.85	kJ/mol	Joback Method
hf	-423.56	kJ/mol	Joback Method
hfus	26.70	kJ/mol	Joback Method
hvap	67.60	kJ/mol	Joback Method
log10ws	-0.20		Aqueous Solubility Prediction Method
logp	-0.556		Crippen Method
mcvol	124.370	ml/mol	McGowan Method

pc	4082.92	kPa	Joback Method
tb	599.21	K	Joback Method
tc	779.81	K	Joback Method
tf	425.90 ± 0.20	K	NIST Webbook
tf	432.39 ± 0.20	K	NIST Webbook
tf	427.65	K	Aqueous Solubility Prediction Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.57	J/mol×K	599.21	Joback Method
cpg	322.72	J/mol×K	629.31	Joback Method
cpg	331.37	J/mol×K	659.41	Joback Method
cpg	339.56	J/mol×K	689.51	Joback Method
cpg	347.29	J/mol×K	719.61	Joback Method
cpg	354.59	J/mol×K	749.71	Joback Method
cpg	361.47	J/mol×K	779.81	Joback Method
hfust	36.97	kJ/mol	431.40	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1596845&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust: Enthalpy of fusion at a given temperature

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