Butanediamide

Other names:	Succindiamide
	Succinic acid diamide
	Succinic amide
	butanedioic acid, diamide
	succinamide
	succinic acid, diamide
	succinic diamide
Inchi:	InChI=1S/C4H8N2O2/c5-3(7)1-2-4(6)8/h1-2H2,(H2,5,7)(H2,6,8)
InchiKey:	SNCZNSNPXMPCGN-UHFFFAOYSA-N
Formula:	C4H8N2O2
SMILES:	NC(=O)CCC(N)=O
Mol. weight [g/mol]:	116.12
CAS:	110-14-5

Physical Properties

Property code	Value	Unit	Source
affp	942.00	kJ/mol	NIST Webbook
chs	-2136.10 ± 2.10	kJ/mol	NIST Webbook
ep	-19.00	J/mol×K	NIST Webbook
gf	-142.14	kJ/mol	Joback Method
hf	-283.47	kJ/mol	Joback Method
hfs	-581.20 ± 2.10	kJ/mol	NIST Webbook
hfus	46.00	kJ/mol	Odd even effect in melting properties of 12 alkane-a,x-diamides
hvap	59.27	kJ/mol	Joback Method
log10ws	0.08		Crippen Method
logp	-1.263		Crippen Method
mcvol	90.320	ml/mol	McGowan Method
pc	5390.71	kPa	Joback Method
tb	543.72	K	Joback Method
tc	761.15	K	Joback Method
tf	401.22	K	Joback Method
vc	0.330	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.78	J/mol×K	688.67	Joback Method
cpg	241.88	J/mol×K	724.91	Joback Method
cpg	207.08	J/mol×K	543.72	Joback Method
cpg	214.93	J/mol×K	579.96	Joback Method
cpg	222.32	J/mol×K	616.20	Joback Method
cpg	229.27	J/mol×K	652.43	Joback Method
cpg	247.57	J/mol×K	761.15	Joback Method
cps	174.00	J/mol×K	323.00	NIST Webbook
hfust	6.08	kJ/mol	485.90	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110145&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Odd even effect in melting properties of 12 alkane-a,x-diamides:	https://www.doi.org/10.1016/j.jct.2006.04.004

Legend

affp:	Proton affinity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
ep:	Protonation entropy at 298K
gf:	Standard Gibbs free energy of formation
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
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