Butanedioic acid, 2,2-dimethyl, diamide

Inchi: InChI=1S/C6H12N2O2/c1-6(2,5(8)10)3-4(7)9/h3H2,1-2H3,(H2,7,9)(H2,8,10)
InchiKey: GETCTGCPPSLAAG-UHFFFAOYSA-N
Formula: C6H12N2O2
SMILES: CC(C)(CC(N)=O)C(N)=O
Mol. weight [g/mol]: 144.17

Physical Properties

Property code	Value	Unit	Source
gf	-122.46	kJ/mol	Joback Method
hf	-333.50	kJ/mol	Joback Method
hfus	17.47	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-0.51		Crippen Method
logp	-0.627		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
rinpol	1195.00		NIST Webbook
rinpol	1195.00		NIST Webbook
tb	586.25	K	Joback Method
tc	809.37	K	Joback Method
tf	426.18	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.95	J/mol×K	586.25	Joback Method
cpg	308.48	J/mol×K	623.44	Joback Method
cpg	318.27	J/mol×K	660.62	Joback Method
cpg	327.35	J/mol×K	697.81	Joback Method
cpg	335.77	J/mol×K	735.00	Joback Method
cpg	343.57	J/mol×K	772.18	Joback Method
cpg	350.79	J/mol×K	809.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R17640&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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