

# Alpha,alpha'-diacetyl-n,n'-di-n-butyl glutaramide

Inchi:	InChI=1S/C17H30N2O4/c1-5-7-9-18-16(22)14(12(3)20)11-15(13(4)21)17(23)19-10-8-6-2
InchiKey:	VIBQIXMERGDODB-UHFFFAOYSA-N
Formula:	C17H30N2O4
SMILES:	CCCCNC(=O)C(CC(C(C)=O)C(=O)NCCCC)C(C)=O
Mol. weight [g/mol]:	326.43
CAS:	93812-81-8

## Physical Properties

Property code	Value	Unit	Source
gf	-249.52	kJ/mol	Joback Method
hf	-748.15	kJ/mol	Joback Method
hfus	49.33	kJ/mol	Joback Method
hvap	92.52	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	1.619		Crippen Method
mcvol	276.630	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
tb	903.30	K	Joback Method
tc	1109.29	K	Joback Method
tf	556.39	K	Joback Method
vc	1.069	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.84	J/molxK	903.30	Joback Method
cpg	904.71	J/molxK	937.63	Joback Method
cpg	917.56	J/molxK	971.96	Joback Method
cpg	929.41	J/molxK	1006.29	Joback Method
cpg	940.31	J/molxK	1040.63	Joback Method
cpg	950.31	J/molxK	1074.96	Joback Method
cpg	959.45	J/molxK	1109.29	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C93812818&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C93812818&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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