

Glutarimide, 3-[(3-methyl-2-oxocyclohexyl)carbonyl]-

Inchi:	InChI=1S/C13H17NO4/c1-7-3-2-4-9(12(7)17)13(18)8-5-10(15)14-11(16)6-8/h7-9H,2-6H2
InchiKey:	FZLLOSYGXMTBHA-UHFFFAOYSA-N
Formula:	C13H17NO4
SMILES:	CC1CCCC(C(=O)C2CC(=O)NC(=O)C2)C1=O
Mol. weight [g/mol]:	251.28
CAS:	92042-21-2

Physical Properties

Property code	Value	Unit	Source
gf	-309.21	kJ/mol	Joback Method
hf	-711.22	kJ/mol	Joback Method
hfus	23.89	kJ/mol	Joback Method
hvap	71.33	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	0.614		Crippen Method
mcvol	188.570	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
tb	837.15	K	Joback Method
tc	1106.63	K	Joback Method
tf	606.41	K	Joback Method
vc	0.693	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.70	J/mol×K	837.15	Joback Method
cpg	649.69	J/mol×K	882.06	Joback Method
cpg	665.13	J/mol×K	926.98	Joback Method
cpg	677.89	J/mol×K	971.89	Joback Method
cpg	687.83	J/mol×K	1016.80	Joback Method
cpg	694.83	J/mol×K	1061.72	Joback Method
cpg	698.75	J/mol×K	1106.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92042212&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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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