

Glutarimide, 3-[2-(3,5-dimethyl-2-oxocyclohexyl)-2-hydroxyethyl] semicarbazone

InChI: InChI=1S/C16H26N4O4/c1-8-3-9(2)15(19-20-16(17)24)11(4-8)12(21)5-10-6-13(22)18-14
InChIKey: NBNURDLSAIQZKM-XDJHFCCHBSA-N

Formula: C16H26N4O4
SMILES: CC1CC(C)C(=NNC(N)=O)C(C(O)CC2CC(=O)NC(=O)C2)C1
Mol. weight [g/mol]: 338.40
CAS: 3428-71-5

Physical Properties

Property code	Value	Unit	Source
hf	-685.00	kJ/mol	Joback Method
hvap	110.96	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	0.497		Crippen Method
mcpvol	260.780	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
tb	1126.90	K	Joback Method
tc	1384.71	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3428715&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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