

Alpha,alpha'-diacetyl-n,n'-dicyclohexyl-glutaramide

Inchi:	InChI=1S/C21H34N2O4/c1-14(24)18(20(26)22-16-9-5-3-6-10-16)13-19(15(2)25)21(27)23
InchiKey:	VBQMOKSUEKZSOD-UHFFFAOYSA-N
Formula:	C21H34N2O4
SMILES:	CC(=O)C(CC(C(C)=O)C(=O)NC1CCCCC1)C(=O)NC1CCCCC1
Mol. weight [g/mol]:	378.51
CAS:	30564-13-7

Physical Properties

Property code	Value	Unit	Source
gf	-166.94	kJ/mol	Joback Method
hf	-722.07	kJ/mol	Joback Method
hfus	43.36	kJ/mol	Joback Method
hvap	102.28	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	2.685		Crippen Method
mcvol	311.270	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
tb	1033.92	K	Joback Method
tc	1272.85	K	Joback Method
tf	616.23	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.78	J/molxK	1033.92	Joback Method
cpg	1130.36	J/molxK	1073.74	Joback Method
cpg	1142.25	J/molxK	1113.56	Joback Method
cpg	1152.56	J/molxK	1153.38	Joback Method
cpg	1161.36	J/molxK	1193.20	Joback Method
cpg	1168.76	J/molxK	1233.02	Joback Method
cpg	1174.83	J/molxK	1272.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30564137&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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