

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

Inchi:	InChI=1S/C23H26N2O4/c1-16(26)20(22(28)24-14-18-9-5-3-6-10-18)13-21(17(2)27)23(29)
InchiKey:	KAMRKTJSEGBHOB-UHFFFAOYSA-N
Formula:	C23H26N2O4
SMILES:	CC(=O)C(CC(C(C)=O)C(=O)NCc1ccccc1)C(=O)NCc1ccccc1
Mol. weight [g/mol]:	394.46
CAS:	95873-08-8

Physical Properties

Property code	Value	Unit	Source
gf	25.82	kJ/mol	Joback Method
hf	-398.93	kJ/mol	Joback Method
hfus	52.96	kJ/mol	Joback Method
hvap	110.42	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	2.420		Crippen Method
mcvol	313.650	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
tb	1093.94	K	Joback Method
tc	1342.36	K	Joback Method
tf	676.85	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.04	J/molxK	1093.94	Joback Method
cpg	1038.48	J/molxK	1135.34	Joback Method
cpg	1047.87	J/molxK	1176.75	Joback Method
cpg	1056.34	J/molxK	1218.15	Joback Method
cpg	1064.01	J/molxK	1259.55	Joback Method
cpg	1071.01	J/molxK	1300.95	Joback Method
cpg	1077.47	J/molxK	1342.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95873088&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

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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