Glutaric acid, monoamide, N-(2-biphenyl)-, isohexyl ester

Inchi: InChI=1S/C23H29NO3/c1-18(2)10-9-17-27-23(26)16-8-15-22(25)24-21-14-7-6-13-20(21)

InchiKey: AKYINDIHZAKQLM-UHFFFAOYSA-N

Formula: C23H29NO3

SMILES: CC(C)CCCOC(=O)CCCC(=O)Nc1ccccc1-c1ccccc1

Mol. weight [g/mol]: 367.48

Physical Properties

Property code	Value	Unit	Source
gf	82.08	kJ/mol	Joback Method
hf	-365.65	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	93.96	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.442		Crippen Method
mcvol	306.400	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	2938.00		NIST Webbook
rinpol	2938.00		NIST Webbook
tb	963.87	K	Joback Method
tc	1190.70	K	Joback Method
tf	574.08	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	986.22	J/mol×K	963.87	Joback Method
cpg	1000.40	J/mol×K	1001.68	Joback Method
cpg	1013.29	J/mol×K	1039.48	Joback Method
cpg	1024.99	J/mol×K	1077.29	Joback Method
cpg	1035.54	J/mol×K	1115.09	Joback Method
cpg	1045.04	J/mol×K	1152.90	Joback Method
cpg	1053.55	J/mol×K	1190.70	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360043&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume