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

Inchi: InChI=1S/C23H29NO3/c1-2-3-4-10-18-27-23(26)17-11-16-22(25)24-21-15-9-8-14-20(21)

InchiKey: UNVWLBKYGVSSHX-UHFFFAOYSA-N

Formula: C23H29NO3

SMILES: CCCCCCOC(=O)CCCC(=O)Nc1ccccc1-c1ccccc1

Mol. weight [g/mol]: 367.48

Physical Properties

Property code	Value	Unit	Source
gf	84.52	kJ/mol	Joback Method
hf	-360.37	kJ/mol	Joback Method
hfus	52.50	kJ/mol	Joback Method
hvap	94.34	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	5.586		Crippen Method
mcvol	306.400	ml/mol	McGowan Method
pc	1416.50	kPa	Joback Method
rinpol	2987.00		NIST Webbook
rinpol	2987.00		NIST Webbook
tb	964.31	K	Joback Method
tc	1189.49	K	Joback Method
tf	589.08	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	985.79	J/mol×K	964.31	Joback Method
cpg	999.92	J/mol×K	1001.84	Joback Method
cpg	1012.81	J/mol×K	1039.37	Joback Method
cpg	1024.51	J/mol×K	1076.90	Joback Method
cpg	1035.12	J/mol×K	1114.43	Joback Method
cpg	1044.69	J/mol×K	1151.96	Joback Method
cpg	1053.30	J/mol×K	1189.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360044&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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