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

Inchi: InChI=1S/C21H25NO3/c1-16(2)15-25-21(24)14-8-13-20(23)22-19-12-7-6-11-18(19)17-9-

InchiKey: BXAJBCPVTYODJR-UHFFFAOYSA-N

Formula: C21H25NO3

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

Mol. weight [g/mol]: 339.43

Physical Properties

Property code	Value	Unit	Source
gf	65.24	kJ/mol	Joback Method
hf	-324.37	kJ/mol	Joback Method
hfus	43.80	kJ/mol	Joback Method
hvap	89.50	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.662		Crippen Method
mcvol	278.220	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	2718.00		NIST Webbook
tb	918.11	K	Joback Method
tc	1145.34	K	Joback Method
tf	551.54	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.91	J/mol×K	918.11	Joback Method
cpg	881.91	J/mol×K	955.98	Joback Method
cpg	894.66	J/mol×K	993.85	Joback Method
cpg	906.22	J/mol×K	1031.73	Joback Method
cpg	916.65	J/mol×K	1069.60	Joback Method
cpg	926.02	J/mol×K	1107.47	Joback Method
cpg	934.39	J/mol×K	1145.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360040&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

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