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

Inchi: InChI=1S/C25H33NO3/c1-2-3-4-5-6-12-20-29-25(28)19-13-18-24(27)26-23-17-11-10-16-

InchiKey: TZMOGKQPOHVLBY-UHFFFAOYSA-N

Formula: C25H33NO3

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

Mol. weight [g/mol]: 395.53

Physical Properties

Property code	Value	Unit	Source
gf	101.36	kJ/mol	Joback Method
hf	-401.65	kJ/mol	Joback Method
hfus	57.68	kJ/mol	Joback Method
hvap	98.80	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	6.366		Crippen Method
mcvol	334.580	ml/mol	McGowan Method
pc	1232.01	kPa	Joback Method
rinpol	3184.00		NIST Webbook
rinpol	3184.00		NIST Webbook
tb	1010.07	K	Joback Method
tc	1239.09	K	Joback Method
tf	611.62	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1106.47	J/mol×K	1010.07	Joback Method
cpg	1120.89	J/mol×K	1048.24	Joback Method
cpg	1134.01	J/mol×K	1086.41	Joback Method
cpg	1145.91	J/mol×K	1124.58	Joback Method
cpg	1156.68	J/mol×K	1162.75	Joback Method
cpg	1166.41	J/mol×K	1200.92	Joback Method
cpg	1175.17	J/mol×K	1239.09	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=U360046&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