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

Inchi: InChI=1S/C29H41NO3/c1-2-3-4-5-6-7-8-9-10-16-24-33-29(32)23-17-22-28(31)30-27-21-
InchiKey: JECBDODISZHFEP-UHFFFAOYSA-N
Formula: C29H41NO3
SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)Nc1ccccc1-c1ccccc1
Mol. weight [g/mol]: 451.64

Physical Properties

Property code	Value	Unit	Source
gf	135.04	kJ/mol	Joback Method
hf	-484.21	kJ/mol	Joback Method
hfus	68.04	kJ/mol	Joback Method
hvap	107.70	kJ/mol	Joback Method
log10ws	-9.42		Crippen Method
logp	7.926		Crippen Method
mcvol	390.940	ml/mol	McGowan Method
pc	956.73	kPa	Joback Method
rinpol	2550.00		NIST Webbook
rinpol	2550.00		NIST Webbook
tb	1101.59	K	Joback Method
tc	1350.70	K	Joback Method
tf	656.70	K	Joback Method
vc	1.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1353.42	J/mol×K	1101.59	Joback Method
cpg	1368.78	J/mol×K	1143.11	Joback Method
cpg	1382.67	J/mol×K	1184.63	Joback Method
cpg	1395.20	J/mol×K	1226.15	Joback Method
cpg	1406.51	J/mol×K	1267.67	Joback Method
cpg	1416.72	J/mol×K	1309.19	Joback Method
cpg	1425.97	J/mol×K	1350.70	Joback Method

Sources

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=U360050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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