

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

Inchi: InChI=1S/C28H39NO3/c1-2-3-4-5-6-7-8-9-15-23-32-28(31)22-16-21-27(30)29-26-20-14-
InchiKey: IGOWNLPHCNQGRI-UHFFFAOYSA-N
Formula: C28H39NO3
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)Nc1ccccc1-c1ccccc1
Mol. weight [g/mol]: 437.61

Physical Properties

Property code	Value	Unit	Source
gf	126.62	kJ/mol	Joback Method
hf	-463.57	kJ/mol	Joback Method
hfus	65.45	kJ/mol	Joback Method
hvap	105.47	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	7.536		Crippen Method
mcvol	376.850	ml/mol	McGowan Method
pc	1016.18	kPa	Joback Method
rinpol	3505.00		NIST Webbook
tb	1078.71	K	Joback Method
tc	1321.07	K	Joback Method
tf	645.43	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1291.07	J/mol×K	1078.71	Joback Method
cpg	1306.14	J/mol×K	1119.10	Joback Method
cpg	1319.78	J/mol×K	1159.50	Joback Method
cpg	1332.11	J/mol×K	1199.89	Joback Method
cpg	1343.24	J/mol×K	1240.29	Joback Method
cpg	1353.30	J/mol×K	1280.68	Joback Method
cpg	1362.38	J/mol×K	1321.07	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=U360049&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
hvac:	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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