

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

Inchi: InChI=1S/C22H27NO3/c1-2-3-9-17-26-22(25)16-10-15-21(24)23-20-14-8-7-13-19(20)18-1
InchiKey: JKASWCKXAHXLHR-UHFFFAOYSA-N
Formula: C22H27NO3
SMILES: CCCCCOC(=O)CCCC(=O)Nc1ccccc1-c1ccccc1
Mol. weight [g/mol]: 353.45

Physical Properties

Property code	Value	Unit	Source
gf	76.10	kJ/mol	Joback Method
hf	-339.73	kJ/mol	Joback Method
hfus	49.91	kJ/mol	Joback Method
hvap	92.12	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.196		Crippen Method
mcvol	292.310	ml/mol	McGowan Method
pc	1524.69	kPa	Joback Method
rinpol	2866.00		NIST Webbook
tb	941.43	K	Joback Method
tc	1166.03	K	Joback Method
tf	577.81	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	926.29	J/mol×K	941.43	Joback Method
cpg	940.30	J/mol×K	978.86	Joback Method
cpg	953.09	J/mol×K	1016.30	Joback Method
cpg	964.71	J/mol×K	1053.73	Joback Method
cpg	975.23	J/mol×K	1091.17	Joback Method
cpg	984.73	J/mol×K	1128.60	Joback Method
cpg	993.26	J/mol×K	1166.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360042&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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