

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

Inchi: InChI=1S/C24H31NO3/c1-2-3-4-5-11-19-28-24(27)18-12-17-23(26)25-22-16-10-9-15-21
InchiKey: OCWKVKPKGUBRDB-UHFFFAOYSA-N
Formula: C24H31NO3
SMILES: CCCCCCOC(=O)CCCC(=O)Nc1ccccc1-c1ccccc1
Mol. weight [g/mol]: 381.51

Physical Properties

Property code	Value	Unit	Source
gf	92.94	kJ/mol	Joback Method
hf	-381.01	kJ/mol	Joback Method
hfus	55.09	kJ/mol	Joback Method
hvap	96.57	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	5.976		Crippen Method
mcvol	320.490	ml/mol	McGowan Method
pc	1319.43	kPa	Joback Method
rinpol	3085.00		NIST Webbook
rinpol	3085.00		NIST Webbook
tb	987.19	K	Joback Method
tc	1213.82	K	Joback Method
tf	600.35	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1045.86	J/mol×K	987.19	Joback Method
cpg	1060.13	J/mol×K	1024.96	Joback Method
cpg	1073.12	J/mol×K	1062.73	Joback Method
cpg	1084.92	J/mol×K	1100.51	Joback Method
cpg	1095.61	J/mol×K	1138.28	Joback Method
cpg	1105.25	J/mol×K	1176.05	Joback Method
cpg	1113.94	J/mol×K	1213.82	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=U360045&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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