

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

Inchi:	InChI=1S/C21H25NO3/c1-2-3-16-25-21(24)15-9-14-20(23)22-19-13-8-7-12-18(19)17-10
InchiKey:	GUUMIVDYGCMINH-UHFFFAOYSA-N
Formula:	C21H25NO3
SMILES:	CCCCOC(=O)CCCC(=O)Nc1ccccc1-c1ccccc1
Mol. weight [g/mol]:	339.43

Physical Properties

Property code	Value	Unit	Source
gf	67.68	kJ/mol	Joback Method
hf	-319.09	kJ/mol	Joback Method
hfus	47.32	kJ/mol	Joback Method
hvap	89.89	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	4.806		Crippen Method
mcvol	278.220	ml/mol	McGowan Method
pc	1645.76	kPa	Joback Method
rinpol	2763.00		NIST Webbook
tb	918.55	K	Joback Method
tc	1143.40	K	Joback Method
tf	566.54	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.41	J/mol×K	918.55	Joback Method
cpg	881.31	J/mol×K	956.02	Joback Method
cpg	894.00	J/mol×K	993.50	Joback Method
cpg	905.52	J/mol×K	1030.97	Joback Method
cpg	915.96	J/mol×K	1068.45	Joback Method
cpg	925.38	J/mol×K	1105.92	Joback Method
cpg	933.83	J/mol×K	1143.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U360041&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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