

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

Inchi: InChI=1S/C20H23NO3/c1-2-15-24-20(23)14-8-13-19(22)21-18-12-7-6-11-17(18)16-9-4-3

InchiKey: OHNWJQSGXIDTRV-UHFFFAOYSA-N

Formula: C20H23NO3

SMILES: CCCOC(=O)CCCC(=O)Nc1ccccc1-c1ccccc1

Mol. weight [g/mol]: 325.40

Physical Properties

Property code	Value	Unit	Source
gf	59.26	kJ/mol	Joback Method
hf	-298.45	kJ/mol	Joback Method
hfus	44.73	kJ/mol	Joback Method
hvap	87.67	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.416		Crippen Method
mcvol	264.130	ml/mol	McGowan Method
pc	1781.84	kPa	Joback Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tb	895.67	K	Joback Method
tc	1121.54	K	Joback Method
tf	555.27	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.21	J/mol×K	895.67	Joback Method
cpg	822.99	J/mol×K	933.31	Joback Method
cpg	835.57	J/mol×K	970.96	Joback Method
cpg	847.00	J/mol×K	1008.60	Joback Method
cpg	857.34	J/mol×K	1046.25	Joback Method
cpg	866.66	J/mol×K	1083.89	Joback Method
cpg	875.01	J/mol×K	1121.54	Joback Method

Sources

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=U360039&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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