

Glutaric acid, monoamide, N,N-di(4-methylphenyl)-, propyl ester

Inchi:	InChI=1S/C22H27NO3/c1-4-16-26-22(25)7-5-6-21(24)23(19-12-8-17(2)9-13-19)20-14-10
InchiKey:	OXQJBVDQTQLTFP-UHFFFAOYSA-N
Formula:	C22H27NO3
SMILES:	CCCOC(=O)CCCC(=O)N(c1ccc(C)cc1)c1ccc(C)cc1
Mol. weight [g/mol]:	353.45

Physical Properties

Property code	Value	Unit	Source
gf	87.86	kJ/mol	Joback Method
hf	-337.14	kJ/mol	Joback Method
hfus	47.45	kJ/mol	Joback Method
hvap	88.39	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.092		Crippen Method
mcvol	292.310	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
rinpol	2702.00		NIST Webbook
rinpol	2702.00		NIST Webbook
tb	908.68	K	Joback Method
tc	1130.21	K	Joback Method
tf	570.14	K	Joback Method
vc	1.099	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.11	J/mol×K	908.68	Joback Method
cpg	926.02	J/mol×K	945.60	Joback Method
cpg	939.70	J/mol×K	982.52	Joback Method
cpg	952.21	J/mol×K	1019.45	Joback Method
cpg	963.63	J/mol×K	1056.37	Joback Method
cpg	974.00	J/mol×K	1093.29	Joback Method
cpg	983.41	J/mol×K	1130.21	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=U360230&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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