Glutaric acid, monoamide, N-(3-methylphenyl)-, undecyl ester

Inchi: InChI=1S/C23H37NO3/c1-3-4-5-6-7-8-9-10-11-18-27-23(26)17-13-16-22(25)24-21-15-12

InchiKey: KDJLTSHWNSBFFX-UHFFFAOYSA-N

Formula: C23H37NO3

SMILES: CCCCCCCCCCCOC(=O)CCCC(=O)Nc1cccc(C)c1

Mol. weight [g/mol]: 375.54

Physical Properties

Property code	Value	Unit	Source
gf	-27.89	kJ/mol	Joback Method
hf	-596.90	kJ/mol	Joback Method
hfus	58.46	kJ/mol	Joback Method
hvap	92.07	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.178		Crippen Method
mcvol	330.160	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	3305.00		NIST Webbook
rinpol	3305.00		NIST Webbook
tb	937.63	K	Joback Method
tc	1148.79	K	Joback Method
tf	562.66	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.26	J/mol×K	937.63	Joback Method
cpg	1105.84	J/mol×K	972.82	Joback Method
cpg	1121.17	J/mol×K	1008.02	Joback Method
cpg	1135.30	J/mol×K	1043.21	Joback Method
cpg	1148.28	J/mol×K	1078.41	Joback Method
cpg	1160.16	J/mol×K	1113.60	Joback Method
cpg	1171.00	J/mol×K	1148.79	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=U360922&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
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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