

Glutaric acid, monoamide, N-(4-methylbenzyl)-, undecyl ester

Inchi: InChI=1S/C24H39NO3/c1-3-4-5-6-7-8-9-10-11-19-28-24(27)14-12-13-23(26)25-20-22-17
InchiKey: KQMKHWMOQNLACQ-UHFFFAOYSA-N
Formula: C24H39NO3
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)NCc1ccc(C)cc1
Mol. weight [g/mol]: 389.57

Physical Properties

Property code	Value	Unit	Source
gf	-19.47	kJ/mol	Joback Method
hf	-617.54	kJ/mol	Joback Method
hfus	61.05	kJ/mol	Joback Method
hvap	94.29	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	5.856		Crippen Method
mcvol	344.250	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	3159.00		NIST Webbook
rinpol	3159.00		NIST Webbook
tb	960.51	K	Joback Method
tc	1175.99	K	Joback Method
tf	573.93	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1150.88	J/mol×K	960.51	Joback Method
cpg	1167.76	J/mol×K	996.42	Joback Method
cpg	1183.34	J/mol×K	1032.34	Joback Method
cpg	1197.65	J/mol×K	1068.25	Joback Method
cpg	1210.76	J/mol×K	1104.16	Joback Method
cpg	1222.74	J/mol×K	1140.07	Joback Method
cpg	1233.63	J/mol×K	1175.99	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U360018&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
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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