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

Inchi: InChI=1S/C27H37NO3/c1-4-5-6-7-8-9-21-31-27(30)12-10-11-26(29)28(24-17-13-22(2)14

InchiKey: IHJBYDGHOBTQDE-UHFFFAOYSA-N

Formula: C27H37NO3

SMILES: CCCCCCCCOC(=O)CCCC(=O)N(c1ccc(C)cc1)c1ccc(C)cc1

Mol. weight [g/mol]: 423.59

Physical Properties

Property code	Value	Unit	Source
gf	129.96	kJ/mol	Joback Method
hf	-440.34	kJ/mol	Joback Method
hfus	60.40	kJ/mol	Joback Method
hvap	99.52	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	7.042		Crippen Method
mcvol	362.760	ml/mol	McGowan Method
pc	1060.33	kPa	Joback Method
rinpol	3204.00		NIST Webbook
rinpol	3204.00		NIST Webbook
tb	1023.08	K	Joback Method
tc	1253.07	K	Joback Method
tf	626.49	K	Joback Method
vc	1.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.82	J/mol×K	1023.08	Joback Method
cpg	1229.45	J/mol×K	1061.41	Joback Method
cpg	1243.72	J/mol×K	1099.74	Joback Method
cpg	1256.74	J/mol×K	1138.08	Joback Method
cpg	1268.60	J/mol×K	1176.41	Joback Method
cpg	1279.39	J/mol×K	1214.74	Joback Method
cpg	1289.20	J/mol×K	1253.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360237&Units=SI
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

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