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

Inchi: InChI=1S/C25H33NO3/c1-4-5-6-7-19-29-25(28)10-8-9-24(27)26(22-15-11-20(2)12-16-22
InchiKey: NHGMZANOUDIFFR-UHFFFAOYSA-N
Formula: C25H33NO3
SMILES: CCCCCCOC(=O)CCCC(=O)N(c1ccc(C)cc1)c1ccc(C)cc1
Mol. weight [g/mol]: 395.53

Physical Properties

Property code	Value	Unit	Source
gf	113.12	kJ/mol	Joback Method
hf	-399.06	kJ/mol	Joback Method
hfus	55.22	kJ/mol	Joback Method
hvap	95.06	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	6.262		Crippen Method
mcvol	334.580	ml/mol	McGowan Method
pc	1206.47	kPa	Joback Method
rinpol	3008.00		NIST Webbook
tb	977.32	K	Joback Method
tc	1201.21	K	Joback Method
tf	603.95	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.10	J/mol×K	977.32	Joback Method
cpg	1106.37	J/mol×K	1014.63	Joback Method
cpg	1120.36	J/mol×K	1051.95	Joback Method
cpg	1133.14	J/mol×K	1089.26	Joback Method
cpg	1144.79	J/mol×K	1126.58	Joback Method
cpg	1155.39	J/mol×K	1163.89	Joback Method
cpg	1165.02	J/mol×K	1201.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360235&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