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

Inchi: InChI=1S/C26H35NO3/c1-4-5-6-7-8-20-30-26(29)11-9-10-25(28)27(23-16-12-21(2)13-17
InchiKey: CDUCEFZEWYEBGA-UHFFFAOYSA-N
Formula: C26H35NO3
SMILES: CCCCCCCOC(=O)CCCC(=O)N(c1ccc(C)cc1)c1ccc(C)cc1
Mol. weight [g/mol]: 409.56

Physical Properties

Property code	Value	Unit	Source
gf	121.54	kJ/mol	Joback Method
hf	-419.70	kJ/mol	Joback Method
hfus	57.81	kJ/mol	Joback Method
hvap	97.29	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	6.652		Crippen Method
mcvol	348.670	ml/mol	McGowan Method
pc	1129.86	kPa	Joback Method
rinpol	3106.00		NIST Webbook
tb	1000.20	K	Joback Method
tc	1226.65	K	Joback Method
tf	615.22	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.21	J/mol×K	1000.20	Joback Method
cpg	1167.65	J/mol×K	1037.94	Joback Method
cpg	1181.77	J/mol×K	1075.68	Joback Method
cpg	1194.66	J/mol×K	1113.42	Joback Method
cpg	1206.40	J/mol×K	1151.17	Joback Method
cpg	1217.09	J/mol×K	1188.91	Joback Method
cpg	1226.80	J/mol×K	1226.65	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=U360236&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume