Glutaric acid, monoamide, N-(4-ethylphenyl)-, dodecyl ester

Inchi: InChI=1S/C25H41NO3/c1-3-5-6-7-8-9-10-11-12-13-21-29-25(28)16-14-15-24(27)26-23-1

InchiKey: MWLDUPSYJWYRSX-UHFFFAOYSA-N

Formula: C25H41NO3

SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)Nc1ccc(CC)cc1

Mol. weight [g/mol]: 403.60

Physical Properties

Property code	Value	Unit	Source
gf	-11.05	kJ/mol	Joback Method
hf	-638.18	kJ/mol	Joback Method
hfus	63.64	kJ/mol	Joback Method
hvap	96.52	kJ/mol	Joback Method
log10ws	-7.62		Crippen Method
logp	6.822		Crippen Method
mcvol	358.340	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	3552.00		NIST Webbook
tb	983.39	K	Joback Method
tc	1204.19	K	Joback Method
tf	585.20	K	Joback Method
vc	1.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.01	J/mol×K	983.39	Joback Method
cpg	1230.24	J/mol×K	1020.19	Joback Method
cpg	1246.07	J/mol×K	1056.99	Joback Method
cpg	1260.58	J/mol×K	1093.79	Joback Method
cpg	1273.84	J/mol×K	1130.59	Joback Method
cpg	1285.91	J/mol×K	1167.39	Joback Method
cpg	1296.85	J/mol×K	1204.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360906&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