Glutaric acid, monoamide, N-(1-phenylethyl)-, dodecyl ester

Inchi: InChI=1S/C25H41NO3/c1-3-4-5-6-7-8-9-10-11-15-21-29-25(28)20-16-19-24(27)26-22(2)
InchiKey: KSZKMEZBMBPFOL-UHFFFAOYSA-N
Formula: C25H41NO3
SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)NC(C)c1ccccc1
Mol. weight [g/mol]: 403.60

Physical Properties

Property code	Value	Unit	Source
gf	-3.86	kJ/mol	Joback Method
hf	-631.99	kJ/mol	Joback Method
hfus	60.51	kJ/mol	Joback Method
hvap	95.47	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.498		Crippen Method
mcvol	358.340	ml/mol	McGowan Method
pc	1003.35	kPa	Joback Method
rinpol	3142.00		NIST Webbook
rinpol	3142.00		NIST Webbook
tb	977.97	K	Joback Method
tc	1197.34	K	Joback Method
tf	557.68	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.98	J/mol×K	977.97	Joback Method
cpg	1231.23	J/mol×K	1014.53	Joback Method
cpg	1247.12	J/mol×K	1051.09	Joback Method
cpg	1261.71	J/mol×K	1087.65	Joback Method
cpg	1275.07	J/mol×K	1124.21	Joback Method
cpg	1287.28	J/mol×K	1160.78	Joback Method
cpg	1298.40	J/mol×K	1197.34	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=U360161&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume