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

Inchi: InChI=1S/C27H45NO3/c1-3-4-5-6-7-8-9-10-11-12-13-17-23-31-27(30)22-18-21-26(29)28
InchiKey: BFLKRBWWPOAYMV-UHFFFAOYSA-N
Formula: C27H45NO3
SMILES: CCCCCCCCCCCCCCOC(=O)CCCC(=O)NC(C)c1ccccc1
Mol. weight [g/mol]: 431.65

Physical Properties

Property code	Value	Unit	Source
gf	12.98	kJ/mol	Joback Method
hf	-673.27	kJ/mol	Joback Method
hfus	65.69	kJ/mol	Joback Method
hvap	99.92	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.278		Crippen Method
mcvol	386.520	ml/mol	McGowan Method
pc	891.60	kPa	Joback Method
rinpol	3338.00		NIST Webbook
rinpol	3338.00		NIST Webbook
tb	1023.73	K	Joback Method
tc	1256.06	K	Joback Method
tf	580.22	K	Joback Method
vc	1.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1339.56	J/mol×K	1023.73	Joback Method
cpg	1357.57	J/mol×K	1062.45	Joback Method
cpg	1374.04	J/mol×K	1101.17	Joback Method
cpg	1389.08	J/mol×K	1139.89	Joback Method
cpg	1402.78	J/mol×K	1178.62	Joback Method
cpg	1415.24	J/mol×K	1217.34	Joback Method
cpg	1426.54	J/mol×K	1256.06	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=U360163&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