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

Inchi: InChI=1S/C21H33NO3/c1-3-4-5-6-7-11-17-25-21(24)16-12-15-20(23)22-18(2)19-13-9-8-
InchiKey: HAGOBEVORYDVOS-UHFFFAOYSA-N
Formula: C21H33NO3
SMILES: CCCCCCCCOC(=O)CCCC(=O)NC(C)c1ccccc1
Mol. weight [g/mol]: 347.49

Physical Properties

Property code	Value	Unit	Source
gf	-37.54	kJ/mol	Joback Method
hf	-549.43	kJ/mol	Joback Method
hfus	50.15	kJ/mol	Joback Method
hvap	86.57	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.938		Crippen Method
mcvol	301.980	ml/mol	McGowan Method
pc	1300.47	kPa	Joback Method
rinpol	2710.00		NIST Webbook
rinpol	2710.00		NIST Webbook
tb	886.45	K	Joback Method
tc	1092.06	K	Joback Method
tf	512.60	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.90	J/mol×K	886.45	Joback Method
cpg	985.10	J/mol×K	920.72	Joback Method
cpg	1000.13	J/mol×K	954.99	Joback Method
cpg	1014.04	J/mol×K	989.26	Joback Method
cpg	1026.88	J/mol×K	1023.52	Joback Method
cpg	1038.70	J/mol×K	1057.79	Joback Method
cpg	1049.55	J/mol×K	1092.06	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=U360158&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