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

Inchi: InChI=1S/C22H35NO3/c1-3-4-5-6-7-8-12-18-26-22(25)17-13-16-21(24)23-19(2)20-14-10

InchiKey: HXUXNYLEBGKTGS-UHFFFAOYSA-N

Formula: C22H35NO3

SMILES: CCCCCCCCCOC(=O)CCCC(=O)NC(C)c1ccccc1

Mol. weight [g/mol]: 361.52

Physical Properties

Property code	Value	Unit	Source
gf	-29.12	kJ/mol	Joback Method
hf	-570.07	kJ/mol	Joback Method
hfus	52.74	kJ/mol	Joback Method
hvap	88.79	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.328		Crippen Method
mcvol	316.070	ml/mol	McGowan Method
pc	1214.90	kPa	Joback Method
rinpol	2809.00		NIST Webbook
rinpol	2809.00		NIST Webbook
tb	909.33	K	Joback Method
tc	1117.03	K	Joback Method
tf	523.87	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.29	J/mol×K	909.33	Joback Method
cpg	1045.71	J/mol×K	943.95	Joback Method
cpg	1060.93	J/mol×K	978.56	Joback Method
cpg	1074.99	J/mol×K	1013.18	Joback Method
cpg	1087.95	J/mol×K	1047.80	Joback Method
cpg	1099.87	J/mol×K	1082.41	Joback Method
cpg	1110.79	J/mol×K	1117.03	Joback Method

Sources

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=U360159&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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