Glutaric acid, monoamide, N-butyl-N-phenyl-, nonyl ester

Inchi: InChI=1S/C24H39NO3/c1-3-5-7-8-9-10-14-21-28-24(27)19-15-18-23(26)25(20-6-4-2)22-
InchiKey: BSWZKFSBYGTXBW-UHFFFAOYSA-N
Formula: C24H39NO3
SMILES: CCCCCCCCCOC(=O)CCCC(=O)N(CCCC)c1ccccc1
Mol. weight [g/mol]: 389.57

Physical Properties

Property code	Value	Unit	Source
gf	11.55	kJ/mol	Joback Method
hf	-592.01	kJ/mol	Joback Method
hfus	59.36	kJ/mol	Joback Method
hvap	89.24	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	6.284		Crippen Method
mcvol	344.250	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	2829.00		NIST Webbook
tb	917.80	K	Joback Method
tc	1124.48	K	Joback Method
tf	541.22	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.27	J/mol×K	917.80	Joback Method
cpg	1151.00	J/mol×K	952.25	Joback Method
cpg	1167.50	J/mol×K	986.69	Joback Method
cpg	1182.82	J/mol×K	1021.14	Joback Method
cpg	1197.04	J/mol×K	1055.59	Joback Method
cpg	1210.21	J/mol×K	1090.04	Joback Method
cpg	1222.40	J/mol×K	1124.48	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=U360178&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