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

Inchi: InChI=1S/C21H33NO3/c1-4-5-16-22(19-12-7-6-8-13-19)20(23)14-9-15-21(24)25-17-10-1

InchiKey: UNZMNTWNFFWOKX-UHFFFAOYSA-N

Formula: C21H33NO3

SMILES: CCCCN(C(=O)CCCC(=O)OCCCC(C)C)c1ccccc1

Mol. weight [g/mol]: 347.49

Physical Properties

Property code	Value	Unit	Source
gf	-16.15	kJ/mol	Joback Method
hf	-535.37	kJ/mol	Joback Method
hfus	48.07	kJ/mol	Joback Method
hvap	82.17	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.969		Crippen Method
mcvol	301.980	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	2504.00		NIST Webbook
rinpol	2504.00		NIST Webbook
tb	848.72	K	Joback Method
tc	1049.18	K	Joback Method
tf	492.41	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.02	J/mol×K	848.72	Joback Method
cpg	968.05	J/mol×K	882.13	Joback Method
cpg	983.93	J/mol×K	915.54	Joback Method
cpg	998.72	J/mol×K	948.95	Joback Method
cpg	1012.46	J/mol×K	982.36	Joback Method
cpg	1025.22	J/mol×K	1015.77	Joback Method
cpg	1037.03	J/mol×K	1049.18	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=U360174&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