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

Inchi: InChI=1S/C33H57NO3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-23-30-37-33(36)28-

InchiKey: GHUUCTIKRACRDB-UHFFFAOYSA-N

Formula: C33H57NO3

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)N(CCCC)c1ccccc1

Mol. weight [g/mol]: 515.81

Physical Properties

Property code	Value	Unit	Source
gf	87.33	kJ/mol	Joback Method
hf	-777.77	kJ/mol	Joback Method
hfus	82.67	kJ/mol	Joback Method
hvap	109.27	kJ/mol	Joback Method
log10ws	-10.48		Crippen Method
logp	9.795		Crippen Method
mcvol	471.060	ml/mol	McGowan Method
pc	641.57	kPa	Joback Method
rinpol	3309.00		NIST Webbook
rinpol	3309.00		NIST Webbook
tb	1123.72	K	Joback Method
tc	1412.30	K	Joback Method
tf	642.65	K	Joback Method
vc	1.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1708.47	J/mol×K	1123.72	Joback Method
cpg	1731.43	J/mol×K	1171.82	Joback Method
cpg	1752.26	J/mol×K	1219.91	Joback Method
cpg	1771.20	J/mol×K	1268.01	Joback Method
cpg	1788.51	J/mol×K	1316.11	Joback Method
cpg	1804.44	J/mol×K	1364.21	Joback Method
cpg	1819.22	J/mol×K	1412.30	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=U360185&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