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

Inchi: InChI=1S/C29H49NO3/c1-3-5-7-8-9-10-11-12-13-14-15-19-26-33-29(32)24-20-23-28(31)
InchiKey: LFVDXMVMJNJMRY-UHFFFAOYSA-N
Formula: C29H49NO3
SMILES: CCCCCCCCCCCCCCOC(=O)CCCC(=O)N(CCCC)c1ccccc1
Mol. weight [g/mol]: 459.70

Physical Properties

Property code	Value	Unit	Source
gf	53.65	kJ/mol	Joback Method
hf	-695.21	kJ/mol	Joback Method
hfus	72.31	kJ/mol	Joback Method
hvap	100.37	kJ/mol	Joback Method
log10ws	-8.81		Crippen Method
logp	8.234		Crippen Method
mcvol	414.700	ml/mol	McGowan Method
pc	787.27	kPa	Joback Method
rinpol	3364.00		NIST Webbook
tb	1032.20	K	Joback Method
tc	1271.29	K	Joback Method
tf	597.57	K	Joback Method
vc	1.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1448.89	J/mol×K	1032.20	Joback Method
cpg	1468.84	J/mol×K	1072.05	Joback Method
cpg	1487.17	J/mol×K	1111.90	Joback Method
cpg	1504.02	J/mol×K	1151.74	Joback Method
cpg	1519.50	J/mol×K	1191.59	Joback Method
cpg	1533.74	J/mol×K	1231.44	Joback Method
cpg	1546.86	J/mol×K	1271.29	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=U360182&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