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

Inchi: InChI=1S/C30H51NO3/c1-3-5-7-8-9-10-11-12-13-14-15-16-20-27-34-30(33)25-21-24-29(

InchiKey: SYQXYOUUYFGBLJ-UHFFFAOYSA-N

Formula: C30H51NO3

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

Mol. weight [g/mol]: 473.73

Physical Properties

Property code	Value	Unit	Source
gf	62.07	kJ/mol	Joback Method
hf	-715.85	kJ/mol	Joback Method
hfus	74.90	kJ/mol	Joback Method
hvap	102.59	kJ/mol	Joback Method
log10ws	-9.23		Crippen Method
logp	8.624		Crippen Method
mcvol	428.790	ml/mol	McGowan Method
pc	746.51	kPa	Joback Method
rinpol	3473.00		NIST Webbook
tb	1055.08	K	Joback Method
tc	1304.28	K	Joback Method
tf	608.84	K	Joback Method
vc	1.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1513.29	J/mol×K	1055.08	Joback Method
cpg	1533.86	J/mol×K	1096.61	Joback Method
cpg	1552.72	J/mol×K	1138.15	Joback Method
cpg	1570.00	J/mol×K	1179.68	Joback Method
cpg	1585.84	J/mol×K	1221.21	Joback Method
cpg	1600.40	J/mol×K	1262.74	Joback Method
cpg	1613.82	J/mol×K	1304.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360183&Units=SI
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

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