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

Inchi: InChI=1S/C27H45NO3/c1-3-5-7-8-9-10-11-12-13-17-24-31-27(30)22-18-21-26(29)28(23-

InchiKey: UGHITWJRKCFUQD-UHFFFAOYSA-N

Formula: C27H45NO3

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

Mol. weight [g/mol]: 431.65

Physical Properties

Property code	Value	Unit	Source
gf	36.81	kJ/mol	Joback Method
hf	-653.93	kJ/mol	Joback Method
hfus	67.13	kJ/mol	Joback Method
hvap	95.92	kJ/mol	Joback Method
log10ws	-7.97		Crippen Method
logp	7.454		Crippen Method
mcvol	386.520	ml/mol	McGowan Method
pc	879.48	kPa	Joback Method
rinpol	3173.00		NIST Webbook
rinpol	3173.00		NIST Webbook
tb	986.44	K	Joback Method
tc	1209.20	K	Joback Method
tf	575.03	K	Joback Method
vc	1.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1321.25	J/mol×K	986.44	Joback Method
cpg	1340.15	J/mol×K	1023.57	Joback Method
cpg	1357.61	J/mol×K	1060.69	Joback Method
cpg	1373.74	J/mol×K	1097.82	Joback Method
cpg	1388.62	J/mol×K	1134.94	Joback Method
cpg	1402.34	J/mol×K	1172.07	Joback Method
cpg	1415.01	J/mol×K	1209.20	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=U360180&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

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