Glutaric acid, monoamide, N-(2-(4-methoxyphenyl)ethyl)-, dodecyl ester

Inchi: InChI=1S/C26H43NO4/c1-3-4-5-6-7-8-9-10-11-12-22-31-26(29)15-13-14-25(28)27-21-20

InchiKey: CCKZXBXISMBMBX-UHFFFAOYSA-N

Formula: C26H43NO4

SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)NCCc1ccc(OC)cc1

Mol. weight [g/mol]: 433.62

Physical Properties

Property code	Value	Unit	Source
gf	-107.63	kJ/mol	Joback Method
hf	-791.04	kJ/mol	Joback Method
hfus	67.42	kJ/mol	Joback Method
hvap	101.16	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	5.988		Crippen Method
mcvol	378.300	ml/mol	McGowan Method
pc	922.18	kPa	Joback Method
rinpol	3515.00		NIST Webbook
tb	1028.69	K	Joback Method
tc	1263.06	K	Joback Method
tf	618.70	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1304.52	J/mol×K	1028.69	Joback Method
cpg	1321.30	J/mol×K	1067.75	Joback Method
cpg	1336.37	J/mol×K	1106.81	Joback Method
cpg	1349.79	J/mol×K	1145.87	Joback Method
cpg	1361.63	J/mol×K	1184.94	Joback Method
cpg	1371.94	J/mol×K	1224.00	Joback Method
cpg	1380.80	J/mol×K	1263.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360227&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

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