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

Inchi: InChI=1S/C24H39NO4/c1-3-4-5-6-7-8-9-10-20-29-24(27)13-11-12-23(26)25-19-18-21-14

InchiKey: YSPQLPGZXQSYHW-UHFFFAOYSA-N

Formula: C24H39NO4

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

Mol. weight [g/mol]: 405.57

Physical Properties

Property code	Value	Unit	Source
gf	-124.47	kJ/mol	Joback Method
hf	-749.76	kJ/mol	Joback Method
hfus	62.24	kJ/mol	Joback Method
hvap	96.70	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.208		Crippen Method
mcvol	350.120	ml/mol	McGowan Method
pc	1039.91	kPa	Joback Method
rinpol	3292.00		NIST Webbook
tb	982.93	K	Joback Method
tc	1203.55	K	Joback Method
tf	596.16	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.16	J/mol×K	982.93	Joback Method
cpg	1196.37	J/mol×K	1019.70	Joback Method
cpg	1211.09	J/mol×K	1056.47	Joback Method
cpg	1224.37	J/mol×K	1093.24	Joback Method
cpg	1236.24	J/mol×K	1130.01	Joback Method
cpg	1246.76	J/mol×K	1166.78	Joback Method
cpg	1255.98	J/mol×K	1203.55	Joback Method

Sources

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=U360226&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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