Glutaric acid, monoamide, N-(4-methoxybenzyl)-, decyl ester

Inchi: InChI=1S/C23H37NO4/c1-3-4-5-6-7-8-9-10-18-28-23(26)13-11-12-22(25)24-19-20-14-16

InchiKey: XUNJXVINLCRUST-UHFFFAOYSA-N

Formula: C23H37NO4

SMILES: CCCCCCCCCCOC(=O)CCCC(=O)NCc1ccc(OC)cc1

Mol. weight [g/mol]: 391.54

Physical Properties

Property code	Value	Unit	Source
gf	-132.89	kJ/mol	Joback Method
hf	-729.12	kJ/mol	Joback Method
hfus	59.65	kJ/mol	Joback Method
hvap	94.48	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.166		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
pc	1107.42	kPa	Joback Method
rinpol	3214.00		NIST Webbook
rinpol	3214.00		NIST Webbook
tb	960.05	K	Joback Method
tc	1175.46	K	Joback Method
tf	584.89	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.61	J/mol×K	960.05	Joback Method
cpg	1134.57	J/mol×K	995.95	Joback Method
cpg	1149.13	J/mol×K	1031.85	Joback Method
cpg	1162.33	J/mol×K	1067.76	Joback Method
cpg	1174.20	J/mol×K	1103.66	Joback Method
cpg	1184.79	J/mol×K	1139.56	Joback Method
cpg	1194.13	J/mol×K	1175.46	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=U360197&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