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

Inchi: InChI=1S/C25H41NO4/c1-3-4-5-6-7-8-9-10-11-12-20-30-25(28)15-13-14-24(27)26-21-22

InchiKey: IGKQWPKTFBLHSZ-UHFFFAOYSA-N

Formula: C25H41NO4

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

Mol. weight [g/mol]: 419.60

Physical Properties

Property code	Value	Unit	Source
gf	-116.05	kJ/mol	Joback Method
hf	-770.40	kJ/mol	Joback Method
hfus	64.83	kJ/mol	Joback Method
hvap	98.93	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	5.946		Crippen Method
mcvol	364.210	ml/mol	McGowan Method
pc	978.40	kPa	Joback Method
rinpol	3417.00		NIST Webbook
tb	1005.81	K	Joback Method
tc	1232.72	K	Joback Method
tf	607.43	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1242.14	J/mol×K	1005.81	Joback Method
cpg	1258.63	J/mol×K	1043.63	Joback Method
cpg	1273.52	J/mol×K	1081.45	Joback Method
cpg	1286.87	J/mol×K	1119.27	Joback Method
cpg	1298.73	J/mol×K	1157.09	Joback Method
cpg	1309.16	J/mol×K	1194.91	Joback Method
cpg	1318.22	J/mol×K	1232.72	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=U360199&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