Glutaric acid, monoamide, N-(2,4-dimethoxyphenyl)-, pentyl ester

Inchi: InChI=1S/C18H27NO5/c1-4-5-6-12-24-18(21)9-7-8-17(20)19-15-11-10-14(22-2)13-16(15

InchiKey: MGZGISCOXBUZEN-UHFFFAOYSA-N

Formula: C18H27NO5

SMILES: CCCCCOC(=O)CCCC(=O)Nc1ccc(OC)cc1OC

Mol. weight [g/mol]: 337.41

Physical Properties

Property code	Value	Unit	Source
gf	-289.62	kJ/mol	Joback Method
hf	-769.61	kJ/mol	Joback Method
hfus	47.50	kJ/mol	Joback Method
hvap	86.42	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.546		Crippen Method
mcvol	271.450	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	3153.00		NIST Webbook
tb	873.05	K	Joback Method
tc	1078.28	K	Joback Method
tf	563.29	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.79	J/mol×K	873.05	Joback Method
cpg	861.08	J/mol×K	907.26	Joback Method
cpg	874.17	J/mol×K	941.46	Joback Method
cpg	886.06	J/mol×K	975.67	Joback Method
cpg	896.75	J/mol×K	1009.87	Joback Method
cpg	906.25	J/mol×K	1044.08	Joback Method
cpg	914.56	J/mol×K	1078.28	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=U360878&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