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

Inchi: InChI=1S/C17H25NO5/c1-4-5-11-23-17(20)8-6-7-16(19)18-14-10-9-13(21-2)12-15(14)22

InchiKey: YZUOPVZSYFYAHV-UHFFFAOYSA-N

Formula: C17H25NO5

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

Mol. weight [g/mol]: 323.38

Physical Properties

Property code	Value	Unit	Source
gf	-298.04	kJ/mol	Joback Method
hf	-748.97	kJ/mol	Joback Method
hfus	44.91	kJ/mol	Joback Method
hvap	84.19	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.156		Crippen Method
mcvol	257.360	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	3061.00		NIST Webbook
tb	850.17	K	Joback Method
tc	1054.65	K	Joback Method
tf	552.02	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.71	J/mol×K	850.17	Joback Method
cpg	802.81	J/mol×K	884.25	Joback Method
cpg	815.77	J/mol×K	918.33	Joback Method
cpg	827.60	J/mol×K	952.41	Joback Method
cpg	838.28	J/mol×K	986.49	Joback Method
cpg	847.82	J/mol×K	1020.57	Joback Method
cpg	856.21	J/mol×K	1054.65	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360877&Units=SI

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