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

Inchi: InChI=1S/C16H23NO5/c1-4-10-22-16(19)7-5-6-15(18)17-13-9-8-12(20-2)11-14(13)21-3/h
InchiKey: AJWYECAYGXHXIQ-UHFFFAOYSA-N
Formula: C16H23NO5
SMILES: CCCOC(=O)CCCC(=O)Nc1ccc(OC)cc1OC
Mol. weight [g/mol]: 309.36

Physical Properties

Property code	Value	Unit	Source
gf	-306.46	kJ/mol	Joback Method
hf	-728.33	kJ/mol	Joback Method
hfus	42.32	kJ/mol	Joback Method
hvap	81.97	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.766		Crippen Method
mcvol	243.270	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpol	2967.00		NIST Webbook
tb	827.29	K	Joback Method
tc	1031.73	K	Joback Method
tf	540.75	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.42	J/mol×K	827.29	Joback Method
cpg	745.31	J/mol×K	861.36	Joback Method
cpg	758.11	J/mol×K	895.44	Joback Method
cpg	769.83	J/mol×K	929.51	Joback Method
cpg	780.46	J/mol×K	963.58	Joback Method
cpg	789.99	J/mol×K	997.65	Joback Method
cpg	798.42	J/mol×K	1031.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360876&Units=SI
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

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