Glutaric acid, 3-methylbut-2-en-1-yl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C18H24O6/c1-13(2)11-12-23-16(19)9-6-10-17(20)24-18-14(21-3)7-5-8-15(18)2

InchiKey: LDAUSDOFRLOBPS-UHFFFAOYSA-N

Formula: C18H24O6

SMILES: COc1cccc(OC)c1OC(=O)CCCC(=O)OCC=C(C)C

Mol. weight [g/mol]: 336.38

Physical Properties

Property code	Value	Unit	Source
gf	-412.34	kJ/mol	Joback Method
hf	-847.87	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	82.43	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.289		Crippen Method
mcvol	263.040	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tb	849.34	K	Joback Method
tc	1057.00	K	Joback Method
tf	513.82	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.70	J/mol×K	849.34	Joback Method
cpg	805.01	J/mol×K	883.95	Joback Method
cpg	818.16	J/mol×K	918.56	Joback Method
cpg	830.16	J/mol×K	953.17	Joback Method
cpg	841.00	J/mol×K	987.78	Joback Method
cpg	850.67	J/mol×K	1022.39	Joback Method
cpg	859.18	J/mol×K	1057.00	Joback Method

Sources

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=U392001&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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