Glutaric acid, 2,6-dimethoxyphenyl isobutyl ester

Inchi: InChI=1S/C17H24O6/c1-12(2)11-22-15(18)9-6-10-16(19)23-17-13(20-3)7-5-8-14(17)21-4

InchiKey: HWXBRDJNUKSPOK-UHFFFAOYSA-N

Formula: C17H24O6

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

Mol. weight [g/mol]: 324.37

Physical Properties

Property code	Value	Unit	Source
gf	-494.87	kJ/mol	Joback Method
hf	-939.94	kJ/mol	Joback Method
hfus	37.48	kJ/mol	Joback Method
hvap	79.78	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.979		Crippen Method
mcvol	253.250	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpol	2357.00		NIST Webbook
rinpol	2357.00		NIST Webbook
tb	821.98	K	Joback Method
tc	1025.45	K	Joback Method
tf	506.59	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.63	J/mol×K	821.98	Joback Method
cpg	775.26	J/mol×K	855.89	Joback Method
cpg	788.73	J/mol×K	889.80	Joback Method
cpg	801.04	J/mol×K	923.72	Joback Method
cpg	812.15	J/mol×K	957.63	Joback Method
cpg	822.06	J/mol×K	991.54	Joback Method
cpg	830.75	J/mol×K	1025.45	Joback Method
dvisc	0.0003812	Pa×s	506.59	Joback Method

dvisc	0.0002242	Pa×s	559.15	Joback Method
dvisc	0.0001444	Pa×s	611.72	Joback Method
dvisc	0.0000998	Pa×s	664.28	Joback Method
dvisc	0.0000727	Pa×s	716.85	Joback Method
dvisc	0.0000554	Pa×s	769.41	Joback Method
dvisc	0.0000437	Pa×s	821.98	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=U358705&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
dvisc:	Dynamic viscosity
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