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

Inchi: InChI=1S/C18H26O6/c1-12(2)13(3)23-16(19)10-7-11-17(20)24-18-14(21-4)8-6-9-15(18)2

InchiKey: JZJWJGRNFFZOBQ-UHFFFAOYSA-N

Formula: C18H26O6

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

Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
gf	-488.89	kJ/mol	Joback Method
hf	-965.86	kJ/mol	Joback Method
hfus	36.54	kJ/mol	Joback Method
hvap	81.62	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.367		Crippen Method
mcvol	267.340	ml/mol	McGowan Method
pc	1512.85	kPa	Joback Method
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook
tb	844.42	K	Joback Method
tc	1049.87	K	Joback Method
tf	502.86	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.86	J/mol×K	844.42	Joback Method
cpg	833.78	J/mol×K	878.66	Joback Method
cpg	847.45	J/mol×K	912.90	Joback Method
cpg	859.85	J/mol×K	947.15	Joback Method
cpg	870.97	J/mol×K	981.39	Joback Method
cpg	880.80	J/mol×K	1015.63	Joback Method
cpg	889.31	J/mol×K	1049.87	Joback Method
dvisc	0.0003864	Pa×s	502.86	Joback Method

dvisc	0.0002110	Pa×s	559.79	Joback Method
dvisc	0.0001288	Pa×s	616.71	Joback Method
dvisc	0.0000855	Pa×s	673.64	Joback Method
dvisc	0.0000605	Pa×s	730.57	Joback Method
dvisc	0.0000450	Pa×s	787.49	Joback Method
dvisc	0.0000348	Pa×s	844.42	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=U391999&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