Glutaric acid, 2,6-dimethoxyphenyl propyl ester

Inchi: InChI=1S/C16H22O6/c1-4-11-21-14(17)9-6-10-15(18)22-16-12(19-2)7-5-8-13(16)20-3/h5

InchiKey: SHMOVALCIDUASW-UHFFFAOYSA-N

Formula: C16H22O6

SMILES: CCCOC(=O)CCCC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 310.34

Physical Properties

Property code	Value	Unit	Source
gf	-500.85	kJ/mol	Joback Method
hf	-914.02	kJ/mol	Joback Method
hfus	38.41	kJ/mol	Joback Method
hvap	77.94	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.733		Crippen Method
mcvol	239.160	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	2299.00		NIST Webbook
rinpol	2299.00		NIST Webbook
tb	799.54	K	Joback Method
tc	1001.20	K	Joback Method
tf	510.32	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.22	J/mol×K	799.54	Joback Method
cpg	763.73	J/mol×K	967.59	Joback Method
cpg	753.82	J/mol×K	933.98	Joback Method
cpg	742.79	J/mol×K	900.37	Joback Method
cpg	730.67	J/mol×K	866.76	Joback Method
cpg	717.47	J/mol×K	833.15	Joback Method
cpg	772.51	J/mol×K	1001.20	Joback Method
dvisc	0.0000545	Pa×s	799.54	Joback Method

dvisc	0.0000678	Pa×s	751.34	Joback Method
dvisc	0.0000870	Pa×s	703.13	Joback Method
dvisc	0.0001158	Pa×s	654.93	Joback Method
dvisc	0.0001612	Pa×s	606.73	Joback Method
dvisc	0.0002376	Pa×s	558.52	Joback Method
dvisc	0.0003770	Pa×s	510.32	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=U358704&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