Glutaric acid, 2,6-dimethoxyphenyl isohexyl ester

Inchi: InChI=1S/C19H28O6/c1-14(2)8-7-13-24-17(20)11-6-12-18(21)25-19-15(22-3)9-5-10-16(1

InchiKey: OPYFHYHSDCSVON-UHFFFAOYSA-N

Formula: C19H28O6

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

Mol. weight [g/mol]: 352.42

Physical Properties

Property code	Value	Unit	Source
gf	-478.03	kJ/mol	Joback Method
hf	-981.22	kJ/mol	Joback Method
hfus	42.66	kJ/mol	Joback Method
hvap	84.23	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.759		Crippen Method
mcvol	281.430	ml/mol	McGowan Method
pc	1397.50	kPa	Joback Method
rinpol	2564.00		NIST Webbook
tb	867.74	K	Joback Method
tc	1071.97	K	Joback Method
tf	529.13	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.78	J/mol×K	867.74	Joback Method
cpg	891.71	J/mol×K	901.78	Joback Method
cpg	905.35	J/mol×K	935.82	Joback Method
cpg	917.69	J/mol×K	969.86	Joback Method
cpg	928.72	J/mol×K	1003.90	Joback Method
cpg	938.43	J/mol×K	1037.93	Joback Method
cpg	946.80	J/mol×K	1071.97	Joback Method
dvisc	0.0003122	Pa×s	529.13	Joback Method
dvisc	0.0001791	Pa×s	585.57	Joback Method

dvisc	0.0001134	Pa×s	642.00	Joback Method
dvisc	0.0000772	Pa×s	698.43	Joback Method
dvisc	0.0000557	Pa×s	754.87	Joback Method
dvisc	0.0000421	Pa×s	811.31	Joback Method
dvisc	0.0000330	Pa×s	867.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358708&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
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