Glutaric acid, 2,6-dimethoxyphenyl pentyl ester

Inchi: InChI=1S/C18H26O6/c1-4-5-6-13-23-16(19)11-8-12-17(20)24-18-14(21-2)9-7-10-15(18)2
InchiKey: BVIOXSQLHIZIMZ-UHFFFAOYSA-N
Formula: C18H26O6
SMILES: CCCCCOC(=O)CCCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
gf	-484.01	kJ/mol	Joback Method
hf	-955.30	kJ/mol	Joback Method
hfus	43.59	kJ/mol	Joback Method
hvap	82.39	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.513		Crippen Method
mcvol	267.340	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	2501.00		NIST Webbook
tb	845.30	K	Joback Method
tc	1046.99	K	Joback Method
tf	532.86	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.79	J/mol×K	845.30	Joback Method
cpg	832.47	J/mol×K	878.92	Joback Method
cpg	845.96	J/mol×K	912.53	Joback Method
cpg	858.25	J/mol×K	946.15	Joback Method
cpg	869.32	J/mol×K	979.76	Joback Method
cpg	879.17	J/mol×K	1013.38	Joback Method
cpg	887.77	J/mol×K	1046.99	Joback Method
dvisc	0.0003135	Pa×s	532.86	Joback Method
dvisc	0.0001926	Pa×s	584.93	Joback Method

dvisc	0.0001281	Pa×s	637.01	Joback Method
dvisc	0.0000906	Pa×s	689.08	Joback Method
dvisc	0.0000673	Pa×s	741.15	Joback Method
dvisc	0.0000520	Pa×s	793.23	Joback Method
dvisc	0.0000415	Pa×s	845.30	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=U358707&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

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