Glutaric acid, 2,6-dimethoxyphenyl octyl ester

Inchi: InChI=1S/C21H32O6/c1-4-5-6-7-8-9-16-26-19(22)14-11-15-20(23)27-21-17(24-2)12-10-1
InchiKey: LMKCALQXARFXSW-UHFFFAOYSA-N
Formula: C21H32O6
SMILES: CCCCCCCCOC(=O)CCCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]: 380.48

Physical Properties

Property code	Value	Unit	Source
gf	-458.75	kJ/mol	Joback Method
hf	-1017.22	kJ/mol	Joback Method
hfus	51.36	kJ/mol	Joback Method
hvap	89.07	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.683		Crippen Method
mcvol	309.610	ml/mol	McGowan Method
pc	1209.83	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	913.94	K	Joback Method
tc	1121.17	K	Joback Method
tf	566.67	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	995.18	J/mol×K	913.94	Joback Method
cpg	1010.29	J/mol×K	948.48	Joback Method
cpg	1023.97	J/mol×K	983.02	Joback Method
cpg	1036.21	J/mol×K	1017.56	Joback Method
cpg	1047.02	J/mol×K	1052.09	Joback Method
cpg	1056.37	J/mol×K	1086.63	Joback Method
cpg	1064.28	J/mol×K	1121.17	Joback Method
dvisc	0.0002304	Pa×s	566.67	Joback Method

dvisc	0.0001366	Pa×s	624.55	Joback Method
dvisc	0.0000884	Pa×s	682.43	Joback Method
dvisc	0.0000613	Pa×s	740.31	Joback Method
dvisc	0.0000448	Pa×s	798.18	Joback Method
dvisc	0.0000342	Pa×s	856.06	Joback Method
dvisc	0.0000270	Pa×s	913.94	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=U358711&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