Glutaric acid, di(2-isopropoxyphenyl) ester

Inchi: InChI=1S/C23H28O6/c1-16(2)26-18-10-5-7-12-20(18)28-22(24)14-9-15-23(25)29-21-13-
InchiKey: MLIWEJSPEVYNME-UHFFFAOYSA-N
Formula: C23H28O6
SMILES: CC(C)Oc1ccccc1OC(=O)CCCC(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 400.46

Physical Properties

Property code	Value	Unit	Source
gf	-334.38	kJ/mol	Joback Method
hf	-832.53	kJ/mol	Joback Method
hfus	43.53	kJ/mol	Joback Method
hvap	95.02	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	4.942		Crippen Method
mcvol	314.030	ml/mol	McGowan Method
pc	1351.64	kPa	Joback Method
rinpol	2872.00		NIST Webbook
rinpol	2872.00		NIST Webbook
tb	985.50	K	Joback Method
tc	1213.94	K	Joback Method
tf	585.63	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.99	J/mol×K	985.50	Joback Method
cpg	1023.34	J/mol×K	1023.57	Joback Method
cpg	1033.95	J/mol×K	1061.65	Joback Method
cpg	1042.81	J/mol×K	1099.72	Joback Method
cpg	1049.95	J/mol×K	1137.79	Joback Method
cpg	1055.36	J/mol×K	1175.86	Joback Method
cpg	1059.06	J/mol×K	1213.94	Joback Method
dvisc	0.0001937	Pa×s	585.63	Joback Method

dvisc	0.0001052	Pa×s	652.27	Joback Method
dvisc	0.0000640	Pa×s	718.92	Joback Method
dvisc	0.0000424	Pa×s	785.57	Joback Method
dvisc	0.0000299	Pa×s	852.21	Joback Method
dvisc	0.0000222	Pa×s	918.86	Joback Method
dvisc	0.0000172	Pa×s	985.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358583&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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