Glutaric acid, dec-2-yl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C24H38O5/c1-5-6-7-8-9-10-14-20(4)28-23(25)17-13-18-24(26)29-22-16-12-11

InchiKey: NIBCUJBTGSWEFZ-UHFFFAOYSA-N

Formula: C24H38O5

SMILES: CCCCCCCCC(C)OC(=O)CCCC(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 406.56

Physical Properties

Property code	Value	Unit	Source
gf	-323.74	kJ/mol	Joback Method
hf	-946.01	kJ/mol	Joback Method
hfus	51.28	kJ/mol	Joback Method
hvap	91.90	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	6.232		Crippen Method
mcvol	346.010	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	2720.00		NIST Webbook
rinpol	2720.00		NIST Webbook
tb	954.30	K	Joback Method
tc	1168.72	K	Joback Method
tf	535.73	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1149.98	J/mol×K	954.30	Joback Method
cpg	1216.20	J/mol×K	1132.98	Joback Method
cpg	1205.97	J/mol×K	1097.25	Joback Method
cpg	1194.26	J/mol×K	1061.51	Joback Method
cpg	1181.04	J/mol×K	1025.77	Joback Method
cpg	1166.29	J/mol×K	990.04	Joback Method
cpg	1224.96	J/mol×K	1168.72	Joback Method
dvisc	0.0000189	Pa×s	954.30	Joback Method

dvisc	0.0000253	Pa×s	884.54	Joback Method
dvisc	0.0000354	Pa×s	814.78	Joback Method
dvisc	0.0000528	Pa×s	745.01	Joback Method
dvisc	0.0000857	Pa×s	675.25	Joback Method
dvisc	0.0001554	Pa×s	605.49	Joback Method
dvisc	0.0003289	Pa×s	535.73	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=U391876&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