Glutaric acid, 2-isopropoxyphenyl hexadecyl ester

Inchi: InChI=1S/C30H50O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-25-33-29(31)23-20-24-30

InchiKey: RXGOPFPPEOECFE-UHFFFAOYSA-N

Formula: C30H50O5

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 490.71

Physical Properties

Property code	Value	Unit	Source
gf	-270.78	kJ/mol	Joback Method
hf	-1064.57	kJ/mol	Joback Method
hfus	70.35	kJ/mol	Joback Method
hvap	105.65	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	8.574		Crippen Method
mcvol	430.550	ml/mol	McGowan Method
pc	730.86	kPa	Joback Method
rinpol	3527.00		NIST Webbook
tb	1092.02	K	Joback Method
tc	1354.95	K	Joback Method
tf	618.35	K	Joback Method
vc	1.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1524.78	J/mol×K	1092.02	Joback Method
cpg	1588.18	J/mol×K	1311.13	Joback Method
cpg	1580.15	J/mol×K	1267.31	Joback Method
cpg	1569.88	J/mol×K	1223.48	Joback Method
cpg	1557.28	J/mol×K	1179.66	Joback Method
cpg	1542.27	J/mol×K	1135.84	Joback Method
cpg	1594.05	J/mol×K	1354.95	Joback Method
dvisc	0.0000081	Pa×s	1092.02	Joback Method
dvisc	0.0000108	Pa×s	1013.07	Joback Method

dvisc	0.0000151	Pa×s	934.13	Joback Method
dvisc	0.0000224	Pa×s	855.18	Joback Method
dvisc	0.0000361	Pa×s	776.24	Joback Method
dvisc	0.0000648	Pa×s	697.29	Joback Method
dvisc	0.0001352	Pa×s	618.35	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=U358582&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