Glutaric acid, 2-isopropoxyphenyl pentadecyl ester

Inchi: InChI=1S/C29H48O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-24-32-28(30)22-19-23-29(31)

InchiKey: KUZFMZGQUKVCNG-UHFFFAOYSA-N

Formula: C29H48O5

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

Mol. weight [g/mol]: 476.69

Physical Properties

Property code	Value	Unit	Source
gf	-279.20	kJ/mol	Joback Method
hf	-1043.93	kJ/mol	Joback Method
hfus	67.76	kJ/mol	Joback Method
hvap	103.42	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	8.184		Crippen Method
mcvol	416.460	ml/mol	McGowan Method
pc	770.32	kPa	Joback Method
rinpol	3417.00		NIST Webbook
tb	1069.14	K	Joback Method
tc	1320.69	K	Joback Method
tf	607.08	K	Joback Method
vc	1.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1461.61	J/mol×K	1069.14	Joback Method
cpg	1478.88	J/mol×K	1111.07	Joback Method
cpg	1493.89	J/mol×K	1152.99	Joback Method
cpg	1506.70	J/mol×K	1194.92	Joback Method
cpg	1517.36	J/mol×K	1236.84	Joback Method
cpg	1525.96	J/mol×K	1278.77	Joback Method
cpg	1532.56	J/mol×K	1320.69	Joback Method
dvisc	0.0001548	Pa×s	607.08	Joback Method
dvisc	0.0000748	Pa×s	684.09	Joback Method

dvisc	0.0000419	Pa×s	761.10	Joback Method
dvisc	0.0000261	Pa×s	838.11	Joback Method
dvisc	0.0000176	Pa×s	915.12	Joback Method
dvisc	0.0000126	Pa×s	992.13	Joback Method
dvisc	0.0000095	Pa×s	1069.14	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U358581&Units=SI

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