Glutaric acid, 3-methylbut-2-yl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C19H28O5/c1-13(2)15(5)23-18(20)11-8-12-19(21)24-17-10-7-6-9-16(17)22-14

InchiKey: JDKGOPKYBKMJFH-UHFFFAOYSA-N

Formula: C19H28O5

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

Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-368.28	kJ/mol	Joback Method
hf	-848.09	kJ/mol	Joback Method
hfus	34.81	kJ/mol	Joback Method
hvap	80.38	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.137		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	2225.00		NIST Webbook
rinpol	2225.00		NIST Webbook
tb	839.46	K	Joback Method
tc	1045.65	K	Joback Method
tf	464.38	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.74	J/mol×K	839.46	Joback Method
cpg	865.60	J/mol×K	873.83	Joback Method
cpg	880.21	J/mol×K	908.19	Joback Method
cpg	893.57	J/mol×K	942.56	Joback Method
cpg	905.69	J/mol×K	976.92	Joback Method
cpg	916.58	J/mol×K	1011.29	Joback Method
cpg	926.26	J/mol×K	1045.65	Joback Method
dvisc	0.0006887	Pa×s	464.38	Joback Method

dvisc	0.0003157	Pa×s	526.89	Joback Method
dvisc	0.0001707	Pa×s	589.41	Joback Method
dvisc	0.0001039	Pa×s	651.92	Joback Method
dvisc	0.0000689	Pa×s	714.43	Joback Method
dvisc	0.0000489	Pa×s	776.95	Joback Method
dvisc	0.0000365	Pa×s	839.46	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=U391867&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