Glutaric acid, 3-methylbut-2-en-1-yl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C19H26O5/c1-14(2)12-13-22-18(20)10-7-11-19(21)24-17-9-6-5-8-16(17)23-15

InchiKey: JCCGAWBYWKYJDK-UHFFFAOYSA-N

Formula: C19H26O5

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

Mol. weight [g/mol]: 334.41

Physical Properties

Property code	Value	Unit	Source
gf	-291.73	kJ/mol	Joback Method
hf	-730.10	kJ/mol	Joback Method
hfus	40.75	kJ/mol	Joback Method
hvap	81.20	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.059		Crippen Method
mcvol	271.260	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpol	2332.00		NIST Webbook
tb	844.38	K	Joback Method
tc	1052.85	K	Joback Method
tf	475.34	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.80	J/mol×K	844.38	Joback Method
cpg	837.04	J/mol×K	879.12	Joback Method
cpg	851.13	J/mol×K	913.87	Joback Method
cpg	864.09	J/mol×K	948.61	Joback Method
cpg	875.93	J/mol×K	983.36	Joback Method
cpg	886.68	J/mol×K	1018.10	Joback Method
cpg	896.37	J/mol×K	1052.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391869&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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

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