Glutaric acid, ethyl 2-isopropylphenyl ester

Inchi: InChI=1S/C16H22O4/c1-4-19-15(17)10-7-11-16(18)20-14-9-6-5-8-13(14)12(2)3/h5-6,8-9
InchiKey: AFEDGQMDZFIZNQ-UHFFFAOYSA-N
Formula: C16H22O4
SMILES: CCOC(=O)CCCC(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]: 278.34

Physical Properties

Property code	Value	Unit	Source
gf	-283.66	kJ/mol	Joback Method
hf	-643.39	kJ/mol	Joback Method
hfus	32.90	kJ/mol	Joback Method
hvap	72.07	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.449		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	1971.00		NIST Webbook
tb	749.28	K	Joback Method
tc	954.00	K	Joback Method
tf	438.34	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.00	J/mol×K	749.28	Joback Method
cpg	664.35	J/mol×K	783.40	Joback Method
cpg	678.69	J/mol×K	817.52	Joback Method
cpg	692.04	J/mol×K	851.64	Joback Method
cpg	704.40	J/mol×K	885.76	Joback Method
cpg	715.80	J/mol×K	919.88	Joback Method
cpg	726.23	J/mol×K	954.00	Joback Method
dvisc	0.0009839	Pa×s	438.34	Joback Method
dvisc	0.0005289	Pa×s	490.16	Joback Method

dvisc	0.0003201	Pa×s	541.99	Joback Method
dvisc	0.0002115	Pa×s	593.81	Joback Method
dvisc	0.0001494	Pa×s	645.63	Joback Method
dvisc	0.0001111	Pa×s	697.46	Joback Method
dvisc	0.0000861	Pa×s	749.28	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U358846&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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