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

Inchi: InChI=1S/C17H24O5/c1-12(2)13(3)21-16(18)10-7-11-17(19)22-15-9-6-5-8-14(15)20-4/h5

InchiKey: HAIAPPAEBAQWGF-UHFFFAOYSA-N

Formula: C17H24O5

SMILES: COc1ccccc1OC(=O)CCCC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 308.37

Physical Properties

Property code	Value	Unit	Source
gf	-382.68	kJ/mol	Joback Method
hf	-801.53	kJ/mol	Joback Method
hfus	33.15	kJ/mol	Joback Method
hvap	76.32	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.359		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2168.00		NIST Webbook
tb	794.14	K	Joback Method
tc	999.34	K	Joback Method
tf	456.84	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.78	J/mol×K	794.14	Joback Method
cpg	749.16	J/mol×K	828.34	Joback Method
cpg	763.42	J/mol×K	862.54	Joback Method
cpg	776.55	J/mol×K	896.74	Joback Method
cpg	788.57	J/mol×K	930.94	Joback Method
cpg	799.47	J/mol×K	965.14	Joback Method
cpg	809.25	J/mol×K	999.34	Joback Method
dvisc	0.0007302	Pa×s	456.84	Joback Method

dvisc	0.0003706	Pa×s	513.06	Joback Method
dvisc	0.0002151	Pa×s	569.27	Joback Method
dvisc	0.0001376	Pa×s	625.49	Joback Method
dvisc	0.0000948	Pa×s	681.71	Joback Method
dvisc	0.0000691	Pa×s	737.92	Joback Method
dvisc	0.0000527	Pa×s	794.14	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=U391754&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