Glutaric acid, 2-methylhex-3-yl 1-phenylethyl ester

Inchi: InChI=1S/C20H30O4/c1-5-10-18(15(2)3)24-20(22)14-9-13-19(21)23-16(4)17-11-7-6-8-12

InchiKey: ASVFVAAPRBILGE-UHFFFAOYSA-N

Formula: C20H30O4

SMILES: CCCC(OC(=O)CCCC(=O)OC(C)c1ccccc1)C(C)C

Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-245.23	kJ/mol	Joback Method
hf	-725.04	kJ/mol	Joback Method
hfus	36.60	kJ/mol	Joback Method
hvap	79.54	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.829		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	2422.00		NIST Webbook
tb	834.94	K	Joback Method
tc	1039.78	K	Joback Method
tf	440.90	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.88	J/mol×K	834.94	Joback Method
cpg	896.53	J/mol×K	869.08	Joback Method
cpg	911.95	J/mol×K	903.22	Joback Method
cpg	926.18	J/mol×K	937.36	Joback Method
cpg	939.24	J/mol×K	971.50	Joback Method
cpg	951.17	J/mol×K	1005.64	Joback Method
cpg	961.99	J/mol×K	1039.78	Joback Method
dvisc	0.0011245	Pa×s	440.90	Joback Method
dvisc	0.0004550	Pa×s	506.57	Joback Method

dvisc	0.0002266	Pa×s	572.25	Joback Method
dvisc	0.0001303	Pa×s	637.92	Joback Method
dvisc	0.0000830	Pa×s	703.59	Joback Method
dvisc	0.0000572	Pa×s	769.27	Joback Method
dvisc	0.0000417	Pa×s	834.94	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=U377515&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