Glutaric acid, isohexyl 1-phenylpropyl ester

Inchi: InChI=1S/C20H30O4/c1-4-18(17-11-6-5-7-12-17)24-20(22)14-8-13-19(21)23-15-9-10-16
InchiKey: HHWNRVHWOZDGKY-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CCC(OC(=O)CCCC(=O)OCCCC(C)C)c1ccccc1
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-242.79	kJ/mol	Joback Method
hf	-719.76	kJ/mol	Joback Method
hfus	40.12	kJ/mol	Joback Method
hvap	79.93	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.831		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2341.00		NIST Webbook
rinpol	2341.00		NIST Webbook
tb	835.38	K	Joback Method
tc	1038.17	K	Joback Method
tf	455.90	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.37	J/mol×K	835.38	Joback Method
cpg	895.86	J/mol×K	869.18	Joback Method
cpg	911.16	J/mol×K	902.98	Joback Method
cpg	925.30	J/mol×K	936.78	Joback Method
cpg	938.31	J/mol×K	970.58	Joback Method
cpg	950.22	J/mol×K	1004.38	Joback Method
cpg	961.05	J/mol×K	1038.17	Joback Method
dvisc	0.0009406	Pa×s	455.90	Joback Method

dvisc	0.0004175	Pa×s	519.15	Joback Method
dvisc	0.0002211	Pa×s	582.39	Joback Method
dvisc	0.0001326	Pa×s	645.64	Joback Method
dvisc	0.0000871	Pa×s	708.89	Joback Method
dvisc	0.0000613	Pa×s	772.13	Joback Method
dvisc	0.0000455	Pa×s	835.38	Joback Method

Sources

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=U358952&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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