Glutaric acid, isohexyl 5-methoxy-3-phenylpentyl ester

Inchi: InChI=1S/C23H36O5/c1-19(2)9-8-16-27-22(24)12-7-13-23(25)28-18-15-21(14-17-26-3)2
InchiKey: ASLXNDLDXPUOHE-UHFFFAOYSA-N
Formula: C23H36O5
SMILES: COCCC(CCOC(=O)CCCC(=O)OCCCC(C)C)c1ccccc1
Mol. weight [g/mol]: 392.53

Physical Properties

Property code	Value	Unit	Source
gf	-322.53	kJ/mol	Joback Method
hf	-913.90	kJ/mol	Joback Method
hfus	49.08	kJ/mol	Joback Method
hvap	89.01	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.890		Crippen Method
mcvol	331.920	ml/mol	McGowan Method
pc	1108.15	kPa	Joback Method
rinpol	2764.00		NIST Webbook
tb	926.44	K	Joback Method
tc	1136.10	K	Joback Method
tf	511.94	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.36	J/mol×K	926.44	Joback Method
cpg	1105.67	J/mol×K	961.38	Joback Method
cpg	1120.53	J/mol×K	996.33	Joback Method
cpg	1133.97	J/mol×K	1031.27	Joback Method
cpg	1146.01	J/mol×K	1066.21	Joback Method
cpg	1156.69	J/mol×K	1101.15	Joback Method
cpg	1166.02	J/mol×K	1136.10	Joback Method
dvisc	0.0004388	Pa×s	511.94	Joback Method
dvisc	0.0001972	Pa×s	581.02	Joback Method

dvisc	0.0001051	Pa×s	650.11	Joback Method
dvisc	0.0000632	Pa×s	719.19	Joback Method
dvisc	0.0000415	Pa×s	788.27	Joback Method
dvisc	0.0000292	Pa×s	857.36	Joback Method
dvisc	0.0000216	Pa×s	926.44	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=U359532&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