Glutaric acid, isobutyl 1-phenyl-2-(3-cyclohexenyl)ethyl ester

Inchi: InChI=1S/C23H32O4/c1-18(2)17-26-22(24)14-9-15-23(25)27-21(20-12-7-4-8-13-20)16-1
InchiKey: TYLDYBBSLXTVSJ-UHFFFAOYSA-N
Formula: C23H32O4
SMILES: CC(C)COC(=O)CCCC(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 372.50

Physical Properties

Property code	Value	Unit	Source
gf	-163.12	kJ/mol	Joback Method
hf	-669.58	kJ/mol	Joback Method
hfus	40.95	kJ/mol	Joback Method
hvap	87.33	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.387		Crippen Method
mcvol	310.890	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	2696.00		NIST Webbook
tb	922.73	K	Joback Method
tc	1144.69	K	Joback Method
tf	497.85	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.76	J/mol×K	922.73	Joback Method
cpg	1041.19	J/mol×K	959.72	Joback Method
cpg	1056.04	J/mol×K	996.72	Joback Method
cpg	1069.37	J/mol×K	1033.71	Joback Method
cpg	1081.23	J/mol×K	1070.71	Joback Method
cpg	1091.68	J/mol×K	1107.70	Joback Method
cpg	1100.75	J/mol×K	1144.69	Joback Method
dvisc	0.0007257	Pa×s	497.85	Joback Method
dvisc	0.0003139	Pa×s	568.66	Joback Method

dvisc	0.0001635	Pa×s	639.48	Joback Method
dvisc	0.0000970	Pa×s	710.29	Joback Method
dvisc	0.0000632	Pa×s	781.10	Joback Method
dvisc	0.0000443	Pa×s	851.92	Joback Method
dvisc	0.0000327	Pa×s	922.73	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=U358585&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