Glutaric acid, 2-methylpent-3-yl 4-biphenyl ester

Inchi: InChI=1S/C23H28O4/c1-4-21(17(2)3)27-23(25)12-8-11-22(24)26-20-15-13-19(14-16-20)18-9-6-5-7-10-18/h5-7,9-10,13-17,21H,4,8,11-12H2,1-3H3

InchiKey: OVTHIPZSDPCSNR-UHFFFAOYSA-N

Formula: C23H28O4

SMILES: CCC(OC(=O)CCCC(=O)Oc1ccc(-c2ccccc2)cc1)C(C)C

Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-114.75	kJ/mol	Joback Method
hf	-556.62	kJ/mol	Joback Method
hfus	41.55	kJ/mol	Joback Method
hvap	89.54	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	5.407		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2837.00		NIST Webbook
rinpol	2837.00		NIST Webbook
tb	935.68	K	Joback Method
tc	1161.36	K	Joback Method
tf	528.65	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.93	J/mol×K	935.68	Joback Method
cpg	1016.97	J/mol×K	1123.75	Joback Method
cpg	1007.80	J/mol×K	1086.13	Joback Method
cpg	997.36	J/mol×K	1048.52	Joback Method
cpg	985.61	J/mol×K	1010.91	Joback Method
cpg	972.48	J/mol×K	973.29	Joback Method
cpg	1024.91	J/mol×K	1161.36	Joback Method
dvisc	0.0000306	Pa×s	935.68	Joback Method

dvisc	0.0000403	Pa×s	867.84	Joback Method
dvisc	0.0000557	Pa×s	800.00	Joback Method
dvisc	0.0000816	Pa×s	732.17	Joback Method
dvisc	0.0001294	Pa×s	664.33	Joback Method
dvisc	0.0002279	Pa×s	596.49	Joback Method
dvisc	0.0004639	Pa×s	528.65	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=U390121&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