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

Inchi: InChI=1S/C22H26O4/c1-16(2)17(3)25-21(23)10-7-11-22(24)26-20-14-12-19(13-15-20)18

InchiKey: JMRHEGMYRWXYPU-UHFFFAOYSA-N

Formula: C22H26O4

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

Mol. weight [g/mol]: 354.44

Physical Properties

Property code	Value	Unit	Source
gf	-123.17	kJ/mol	Joback Method
hf	-535.98	kJ/mol	Joback Method
hfus	38.96	kJ/mol	Joback Method
hvap	87.32	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.017		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	912.80	K	Joback Method
tc	1139.10	K	Joback Method
tf	517.38	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.83	J/mol×K	912.80	Joback Method
cpg	913.38	J/mol×K	950.52	Joback Method
cpg	926.53	J/mol×K	988.23	Joback Method
cpg	938.32	J/mol×K	1025.95	Joback Method
cpg	948.81	J/mol×K	1063.67	Joback Method
cpg	958.04	J/mol×K	1101.39	Joback Method
cpg	966.05	J/mol×K	1139.10	Joback Method
dvisc	0.0005200	Pa×s	517.38	Joback Method

dvisc	0.0002580	Pa×s	583.28	Joback Method
dvisc	0.0001476	Pa×s	649.19	Joback Method
dvisc	0.0000936	Pa×s	715.09	Joback Method
dvisc	0.0000641	Pa×s	780.99	Joback Method
dvisc	0.0000465	Pa×s	846.90	Joback Method
dvisc	0.0000354	Pa×s	912.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390120&Units=SI
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

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