Glutaric acid, di(2-tert-butyl-6-methylphenyl) ester

Inchi: InChI=1S/C27H36O4/c1-18-12-9-14-20(26(3,4)5)24(18)30-22(28)16-11-17-23(29)31-25-

InchiKey: YHRFTVXYANLGBC-UHFFFAOYSA-N

Formula: C27H36O4

SMILES: Cc1cccc(C(C)(C)C)c1OC(=O)CCCC(=O)Oc1c(C)cccc1C(C)(C)C

Mol. weight [g/mol]: 424.57

Physical Properties

Property code	Value	Unit	Source
gf	-99.40	kJ/mol	Joback Method
hf	-680.53	kJ/mol	Joback Method
hfus	42.96	kJ/mol	Joback Method
hvap	98.62	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	6.580		Crippen Method
mcvol	358.650	ml/mol	McGowan Method
pc	1055.51	kPa	Joback Method
rinpol	3069.00		NIST Webbook
rinpol	3069.00		NIST Webbook
tb	1036.56	K	Joback Method
tc	1273.76	K	Joback Method
tf	646.13	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1196.06	J/mol×K	1036.56	Joback Method
cpg	1210.92	J/mol×K	1076.09	Joback Method
cpg	1224.44	J/mol×K	1115.63	Joback Method
cpg	1236.73	J/mol×K	1155.16	Joback Method
cpg	1247.89	J/mol×K	1194.69	Joback Method
cpg	1258.02	J/mol×K	1234.22	Joback Method
cpg	1267.23	J/mol×K	1273.76	Joback Method
dvisc	0.0001219	Pa×s	646.13	Joback Method

dvisc	0.0000699	Pa×s	711.20	Joback Method
dvisc	0.0000440	Pa×s	776.27	Joback Method
dvisc	0.0000297	Pa×s	841.35	Joback Method
dvisc	0.0000212	Pa×s	906.42	Joback Method
dvisc	0.0000159	Pa×s	971.49	Joback Method
dvisc	0.0000123	Pa×s	1036.56	Joback Method

Sources

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=U359140&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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