Glutaric acid, isobutyl 2-tert-butyl-6-methylphenyl ester

Inchi: InChI=1S/C20H30O4/c1-14(2)13-23-17(21)11-8-12-18(22)24-19-15(3)9-7-10-16(19)20(4

InchiKey: CYBUQWKLVCIIFA-UHFFFAOYSA-N

Formula: C20H30O4

SMILES: Cc1cccc(C(C)(C)C)c1OC(=O)CCCC(=O)OCC(C)C

Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-256.77	kJ/mol	Joback Method
hf	-746.17	kJ/mol	Joback Method
hfus	35.46	kJ/mol	Joback Method
hvap	80.34	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.567		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
rinpol	2350.00		NIST Webbook
tb	842.55	K	Joback Method
tc	1050.69	K	Joback Method
tf	498.36	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.59	J/mol×K	842.55	Joback Method
cpg	894.95	J/mol×K	877.24	Joback Method
cpg	910.13	J/mol×K	911.93	Joback Method
cpg	924.16	J/mol×K	946.62	Joback Method
cpg	937.07	J/mol×K	981.31	Joback Method
cpg	948.92	J/mol×K	1016.00	Joback Method
cpg	959.72	J/mol×K	1050.69	Joback Method
dvisc	0.0005272	Pa×s	498.36	Joback Method
dvisc	0.0002752	Pa×s	555.72	Joback Method

dvisc	0.0001622	Pa×s	613.09	Joback Method
dvisc	0.0001046	Pa×s	670.45	Joback Method
dvisc	0.0000724	Pa×s	727.82	Joback Method
dvisc	0.0000528	Pa×s	785.18	Joback Method
dvisc	0.0000402	Pa×s	842.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359134&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