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

Inchi: InChI=1S/C23H36O4/c1-6-7-8-9-10-17-26-20(24)15-12-16-21(25)27-22-18(2)13-11-14-1

InchiKey: ZRXONTRGBDSFRM-UHFFFAOYSA-N

Formula: C23H36O4

SMILES: CCCCCCCOC(=O)CCCC(=O)Oc1c(C)cccc1C(C)(C)C

Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-229.07	kJ/mol	Joback Method
hf	-802.81	kJ/mol	Joback Method
hfus	46.75	kJ/mol	Joback Method
hvap	87.41	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.882		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1100.81	kPa	Joback Method
rinpol	2663.00		NIST Webbook
rinpol	2663.00		NIST Webbook
tb	911.63	K	Joback Method
tc	1120.72	K	Joback Method
tf	547.17	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.83	J/mol×K	911.63	Joback Method
cpg	1129.34	J/mol×K	1085.87	Joback Method
cpg	1117.38	J/mol×K	1051.02	Joback Method
cpg	1104.29	J/mol×K	1016.18	Joback Method
cpg	1090.03	J/mol×K	981.33	Joback Method
cpg	1074.56	J/mol×K	946.48	Joback Method
cpg	1140.24	J/mol×K	1120.72	Joback Method
dvisc	0.0000281	Pa×s	911.63	Joback Method

dvisc	0.0000366	Pa×s	850.89	Joback Method
dvisc	0.0000497	Pa×s	790.14	Joback Method
dvisc	0.0000710	Pa×s	729.40	Joback Method
dvisc	0.0001083	Pa×s	668.66	Joback Method
dvisc	0.0001795	Pa×s	607.91	Joback Method
dvisc	0.0003331	Pa×s	547.17	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=U359138&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