Glutaric acid, 2-ethylhexyl cis-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C23H42O4/c1-6-8-10-18(7-2)17-26-21(24)11-9-12-22(25)27-20-15-13-19(14-1

InchiKey: LPHMDBAIUWSUBJ-UHFFFAOYSA-N

Formula: C23H42O4

SMILES: CCCCC(CC)COC(=O)CCCC(=O)OC1CCC(C(C)(C)C)CC1

Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	-307.92	kJ/mol	Joback Method
hf	-987.70	kJ/mol	Joback Method
hfus	42.87	kJ/mol	Joback Method
hvap	83.54	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	6.064		Crippen Method
mcvol	338.950	ml/mol	McGowan Method
pc	1017.48	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	889.43	K	Joback Method
tc	1094.35	K	Joback Method
tf	483.85	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.24	J/mol×K	889.43	Joback Method
cpg	1175.97	J/mol×K	923.58	Joback Method
cpg	1194.18	J/mol×K	957.74	Joback Method
cpg	1210.93	J/mol×K	991.89	Joback Method
cpg	1226.26	J/mol×K	1026.04	Joback Method
cpg	1240.20	J/mol×K	1060.20	Joback Method
cpg	1252.81	J/mol×K	1094.35	Joback Method
dvisc	0.0007849	Pa×s	483.85	Joback Method

dvisc	0.0003344	Pa×s	551.45	Joback Method
dvisc	0.0001717	Pa×s	619.04	Joback Method
dvisc	0.0001005	Pa×s	686.64	Joback Method
dvisc	0.0000647	Pa×s	754.24	Joback Method
dvisc	0.0000448	Pa×s	821.83	Joback Method
dvisc	0.0000328	Pa×s	889.43	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=U393389&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