Glutaric acid, 2-methylpent-3-yl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C21H38O4/c1-7-18(15(2)3)25-20(23)10-8-9-19(22)24-17-13-11-16(12-14-17)2

InchiKey: QVZJCFNTXDRNQP-UHFFFAOYSA-N

Formula: C21H38O4

SMILES: CCC(OC(=O)CCCC(=O)OC1CCC(C(C)(C)C)CC1)C(C)C

Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-327.20	kJ/mol	Joback Method
hf	-951.70	kJ/mol	Joback Method
hfus	34.17	kJ/mol	Joback Method
hvap	78.70	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.283		Crippen Method
mcvol	310.770	ml/mol	McGowan Method
pc	1160.87	kPa	Joback Method
rinpol	2356.00		NIST Webbook
rinpol	2356.00		NIST Webbook
tb	843.23	K	Joback Method
tc	1047.53	K	Joback Method
tf	446.31	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.49	J/mol×K	843.23	Joback Method
cpg	1052.36	J/mol×K	877.28	Joback Method
cpg	1070.75	J/mol×K	911.33	Joback Method
cpg	1087.72	J/mol×K	945.38	Joback Method
cpg	1103.30	J/mol×K	979.43	Joback Method
cpg	1117.53	J/mol×K	1013.48	Joback Method
cpg	1130.44	J/mol×K	1047.53	Joback Method
dvisc	0.0012139	Pa×s	446.31	Joback Method

dvisc	0.0004787	Pa×s	512.46	Joback Method
dvisc	0.0002335	Pa×s	578.62	Joback Method
dvisc	0.0001320	Pa×s	644.77	Joback Method
dvisc	0.0000830	Pa×s	710.92	Joback Method
dvisc	0.0000564	Pa×s	777.08	Joback Method
dvisc	0.0000408	Pa×s	843.23	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=U393401&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

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