Glutaric acid, 1-(tert-butoxy)prop-2-yl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H34O5/c1-8-15(13(2)3)23-17(20)11-9-10-16(19)22-14(4)12-21-18(5,6)7/h1

InchiKey: UKMCUZARQKHXPY-UHFFFAOYSA-N

Formula: C18H34O5

SMILES: CCC(OC(=O)CCCC(=O)OC(C)COC(C)(C)C)C(C)C

Mol. weight [g/mol]: 330.46

Physical Properties

Property code	Value	Unit	Source
gf	-476.64	kJ/mol	Joback Method
hf	-1061.26	kJ/mol	Joback Method
hfus	31.15	kJ/mol	Joback Method
hvap	73.92	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.881		Crippen Method
mcvol	285.230	ml/mol	McGowan Method
pc	1250.38	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	781.69	K	Joback Method
tc	970.61	K	Joback Method
tf	416.59	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.31	J/mol×K	781.69	Joback Method
cpg	901.04	J/mol×K	813.18	Joback Method
cpg	917.69	J/mol×K	844.66	Joback Method
cpg	933.27	J/mol×K	876.15	Joback Method
cpg	947.81	J/mol×K	907.64	Joback Method
cpg	961.32	J/mol×K	939.13	Joback Method
cpg	973.82	J/mol×K	970.61	Joback Method
dvisc	0.0012371	Pa×s	416.59	Joback Method

dvisc	0.0004622	Pa×s	477.44	Joback Method
dvisc	0.0002158	Pa×s	538.29	Joback Method
dvisc	0.0001176	Pa×s	599.14	Joback Method
dvisc	0.0000717	Pa×s	659.99	Joback Method
dvisc	0.0000475	Pa×s	720.84	Joback Method
dvisc	0.0000335	Pa×s	781.69	Joback Method

Sources

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=U380532&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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