Glutaric acid, oct-1-en-3-yl 3-methylbut-2-yl ester

Inchi: InChI=1S/C18H32O4/c1-6-8-9-11-16(7-2)22-18(20)13-10-12-17(19)21-15(5)14(3)4/h7,14

InchiKey: FNLWZXMRLDNAGU-UHFFFAOYSA-N

Formula: C18H32O4

SMILES: C=CC(CCCCC)OC(=O)CCCC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-286.64	kJ/mol	Joback Method
hf	-794.86	kJ/mol	Joback Method
hfus	36.10	kJ/mol	Joback Method
hvap	72.14	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.423		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	759.18	K	Joback Method
tc	943.63	K	Joback Method
tf	390.18	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.17	J/mol×K	759.18	Joback Method
cpg	842.53	J/mol×K	789.92	Joback Method
cpg	858.93	J/mol×K	820.66	Joback Method
cpg	874.38	J/mol×K	851.41	Joback Method
cpg	888.88	J/mol×K	882.15	Joback Method
cpg	902.47	J/mol×K	912.89	Joback Method
cpg	915.15	J/mol×K	943.63	Joback Method
dvisc	0.0018969	Pa×s	390.18	Joback Method

dvisc	0.0007164	Pa×s	451.68	Joback Method
dvisc	0.0003417	Pa×s	513.18	Joback Method
dvisc	0.0001910	Pa×s	574.68	Joback Method
dvisc	0.0001194	Pa×s	636.18	Joback Method
dvisc	0.0000811	Pa×s	697.68	Joback Method
dvisc	0.0000587	Pa×s	759.18	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=U405346&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