Glutaric acid, 3-methylbut-2-yl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C17H32O5/c1-13(2)15(4)22-17(19)8-6-7-16(18)21-12-10-14(3)9-11-20-5/h13-1

InchiKey: ZSUAXNXPPVZXRR-UHFFFAOYSA-N

Formula: C17H32O5

SMILES: COCCC(C)CCOC(=O)CCCC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 316.43

Physical Properties

Property code	Value	Unit	Source
gf	-487.90	kJ/mol	Joback Method
hf	-1031.87	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	72.99	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.350		Crippen Method
mcvol	271.140	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook
tb	762.04	K	Joback Method
tc	945.49	K	Joback Method
tf	402.90	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.06	J/mol×K	762.04	Joback Method
cpg	840.31	J/mol×K	792.62	Joback Method
cpg	856.57	J/mol×K	823.19	Joback Method
cpg	871.87	J/mol×K	853.77	Joback Method
cpg	886.18	J/mol×K	884.34	Joback Method
cpg	899.52	J/mol×K	914.92	Joback Method
cpg	911.89	J/mol×K	945.49	Joback Method
dvisc	0.0013968	Pa×s	402.90	Joback Method

dvisc	0.0005535	Pa×s	462.76	Joback Method
dvisc	0.0002711	Pa×s	522.61	Joback Method
dvisc	0.0001538	Pa×s	582.47	Joback Method
dvisc	0.0000970	Pa×s	642.33	Joback Method
dvisc	0.0000661	Pa×s	702.18	Joback Method
dvisc	0.0000479	Pa×s	762.04	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=U393518&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