Glutaric acid, 2-methylpent-3-yl but-3-en-1-yl ester

Inchi: InChI=1S/C15H26O4/c1-5-7-11-18-14(16)9-8-10-15(17)19-13(6-2)12(3)4/h5,12-13H,1,6-

InchiKey: NPAXMPOJQBPKGM-UHFFFAOYSA-N

Formula: C15H26O4

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

Mol. weight [g/mol]: 270.36

Physical Properties

Property code	Value	Unit	Source
gf	-309.46	kJ/mol	Joback Method
hf	-727.66	kJ/mol	Joback Method
hfus	31.85	kJ/mol	Joback Method
hvap	65.85	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.254		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	1702.00		NIST Webbook
rinpol	1702.00		NIST Webbook
tb	690.98	K	Joback Method
tc	873.40	K	Joback Method
tf	371.37	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.33	J/mol×K	690.98	Joback Method
cpg	670.39	J/mol×K	721.38	Joback Method
cpg	685.64	J/mol×K	751.79	Joback Method
cpg	700.07	J/mol×K	782.19	Joback Method
cpg	713.72	J/mol×K	812.59	Joback Method
cpg	726.57	J/mol×K	842.99	Joback Method
cpg	738.65	J/mol×K	873.40	Joback Method
dvisc	0.0020674	Pa×s	371.37	Joback Method

dvisc	0.0008976	Pa×s	424.64	Joback Method
dvisc	0.0004694	Pa×s	477.91	Joback Method
dvisc	0.0002795	Pa×s	531.17	Joback Method
dvisc	0.0001830	Pa×s	584.44	Joback Method
dvisc	0.0001286	Pa×s	637.71	Joback Method
dvisc	0.0000954	Pa×s	690.98	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=U394032&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