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

Inchi: InChI=1S/C14H22O4/c1-5-12(4)18-14(16)8-6-7-13(15)17-10-9-11(2)3/h5,9,12H,1,6-8,10
InchiKey: PWODKIGQXUCRBJ-UHFFFAOYSA-N
Formula: C14H22O4
SMILES: C=CC(C)OC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	-243.77	kJ/mol	Joback Method
hf	-594.31	kJ/mol	Joback Method
hfus	31.68	kJ/mol	Joback Method
hvap	64.05	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.784		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	1666.00		NIST Webbook
rinpol	1666.00		NIST Webbook
tb	672.58	K	Joback Method
tc	861.42	K	Joback Method
tf	356.06	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.06	J/mol×K	672.58	Joback Method
cpg	592.09	J/mol×K	704.05	Joback Method
cpg	606.35	J/mol×K	735.53	Joback Method
cpg	619.84	J/mol×K	767.00	Joback Method
cpg	632.59	J/mol×K	798.47	Joback Method
cpg	644.62	J/mol×K	829.95	Joback Method
cpg	655.94	J/mol×K	861.42	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=U405234&Units=SI

Legend

cpg:	Ideal gas heat capacity
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