2-(2-Butenylidene)-3,3-dimethyl-5-(2-oxopropyl)te diastereomer 1

Inchi: InChI=1S/C13H20O2/c1-5-6-7-12-13(3,4)9-11(15-12)8-10(2)14/h5-7,11H,8-9H2,1-4H3/b
InchiKey: SUQDFKVIGVYZSR-QYHKEWNESA-N
Formula: C13H20O2
SMILES: CC=CC=C1OC(CC(C)=O)CC1(C)C
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-7.43	kJ/mol	Joback Method
hf	-307.60	kJ/mol	Joback Method
hfus	28.24	kJ/mol	Joback Method
hvap	55.33	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.241		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
ripol	2094.00		NIST Webbook
ripol	2094.00		NIST Webbook
tb	599.31	K	Joback Method
tc	811.63	K	Joback Method
tf	348.61	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.91	J/mol×K	599.31	Joback Method
cpg	487.10	J/mol×K	634.70	Joback Method
cpg	503.33	J/mol×K	670.08	Joback Method
cpg	518.71	J/mol×K	705.47	Joback Method
cpg	533.39	J/mol×K	740.85	Joback Method
cpg	547.47	J/mol×K	776.24	Joback Method
cpg	561.10	J/mol×K	811.63	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=R495375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume