Succinic acid, isobutyl 3-methylbut-3-enyl ester

Inchi: InChI=1S/C13H22O4/c1-10(2)7-8-16-12(14)5-6-13(15)17-9-11(3)4/h11H,1,5-9H2,2-4H3
InchiKey: WXWCOSOHWCHPTP-UHFFFAOYSA-N
Formula: C13H22O4
SMILES: C=C(C)CCOC(=O)CCC(=O)OCC(C)C
Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	-332.41	kJ/mol	Joback Method
hf	-690.89	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	61.87	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.475		Crippen Method
mcvol	204.610	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1582.00		NIST Webbook
tb	645.54	K	Joback Method
tc	829.62	K	Joback Method
tf	349.87	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.01	J/mol×K	645.54	Joback Method
cpg	561.03	J/mol×K	676.22	Joback Method
cpg	575.32	J/mol×K	706.90	Joback Method
cpg	588.91	J/mol×K	737.58	Joback Method
cpg	601.79	J/mol×K	768.26	Joback Method
cpg	613.96	J/mol×K	798.94	Joback Method
cpg	625.44	J/mol×K	829.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353440&Units=SI
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

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