Succinic acid, 3-methylbut-2-yl 3-methylbut-3-en-1-yl ester

Inchi: InChI=1S/C14H24O4/c1-10(2)8-9-17-13(15)6-7-14(16)18-12(5)11(3)4/h11-12H,1,6-9H2,

InchiKey: YBDHYBXHGSIZTH-UHFFFAOYSA-N

Formula: C14H24O4

SMILES: C=C(C)CCOC(=O)CCC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	-326.43	kJ/mol	Joback Method
hf	-716.81	kJ/mol	Joback Method
hfus	27.95	kJ/mol	Joback Method
hvap	63.70	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.864		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
tb	667.98	K	Joback Method
tc	853.60	K	Joback Method
tf	346.14	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.58	J/mol×K	667.98	Joback Method
cpg	615.37	J/mol×K	698.92	Joback Method
cpg	630.37	J/mol×K	729.85	Joback Method
cpg	644.59	J/mol×K	760.79	Joback Method
cpg	658.03	J/mol×K	791.73	Joback Method
cpg	670.70	J/mol×K	822.66	Joback Method
cpg	682.61	J/mol×K	853.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391132&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