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

Inchi: InChI=1S/C14H24O4/c1-10(2)8-9-17-13(15)6-7-14(16)18-12(5)11(3)4/h8,11-12H,6-7,9H2

InchiKey: KXLCDHQOKYYBPH-UHFFFAOYSA-N

Formula: C14H24O4

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

Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	-334.05	kJ/mol	Joback Method
hf	-725.02	kJ/mol	Joback Method
hfus	29.44	kJ/mol	Joback Method
hvap	64.33	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.864		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	1668.00		NIST Webbook
rinpol	1668.00		NIST Webbook
tb	675.46	K	Joback Method
tc	864.48	K	Joback Method
tf	342.82	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.77	J/mol×K	675.46	Joback Method
cpg	616.61	J/mol×K	706.96	Joback Method
cpg	631.64	J/mol×K	738.47	Joback Method
cpg	645.87	J/mol×K	769.97	Joback Method
cpg	659.31	J/mol×K	801.47	Joback Method
cpg	671.98	J/mol×K	832.98	Joback Method
cpg	683.90	J/mol×K	864.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390581&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

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