

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

Inchi:	InChI=1S/C11H18O4/c1-4-14-10(12)5-6-11(13)15-8-7-9(2)3/h2,4-8H2,1,3H3
InchiKey:	IQJGVZUEKIBIOA-UHFFFAOYSA-N
Formula:	C11H18O4
SMILES:	<chem>C=C(C)CCOC(=O)CCC(=O)OCC</chem>
Mol. weight [g/mol]:	214.26

Physical Properties

Property code	Value	Unit	Source
gf	-346.81	kJ/mol	Joback Method
hf	-644.33	kJ/mol	Joback Method
hfus	27.23	kJ/mol	Joback Method
hvap	57.80	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.839		Crippen Method
mcvol	176.430	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinsol	1456.00		NIST Webbook
tb	600.22	K	Joback Method
tc	784.41	K	Joback Method
tf	342.33	K	Joback Method
vc	0.681	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.71	J/mol×K	600.22	Joback Method
cpg	457.22	J/mol×K	630.92	Joback Method
cpg	470.12	J/mol×K	661.62	Joback Method
cpg	482.43	J/mol×K	692.32	Joback Method
cpg	494.14	J/mol×K	723.01	Joback Method
cpg	505.25	J/mol×K	753.71	Joback Method
cpg	515.77	J/mol×K	784.41	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=U353438&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
mccvol:	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

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