

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

Inchi:	InChI=1S/C11H16Cl2O4/c1-8(2)5-6-16-10(14)3-4-11(15)17-7-9(12)13/h9H,1,3-7H2,2H3
InchiKey:	OLEUXFIBVUKTLN-UHFFFAOYSA-N
Formula:	C11H16Cl2O4
SMILES:	C=C(C)CCOC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	283.15

Physical Properties

Property code	Value	Unit	Source
gf	-373.11	kJ/mol	Joback Method
hf	-681.09	kJ/mol	Joback Method
hfus	32.10	kJ/mol	Joback Method
hvap	66.18	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.623		Crippen Method
mvol	200.910	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1768.00		NIST Webbook
rinpol	1768.00		NIST Webbook
tb	674.64	K	Joback Method
tc	870.24	K	Joback Method
tf	387.17	K	Joback Method
vc	0.773	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.00	J/mol×K	674.64	Joback Method
cpg	510.26	J/mol×K	707.24	Joback Method
cpg	521.82	J/mol×K	739.84	Joback Method
cpg	532.70	J/mol×K	772.44	Joback Method
cpg	542.90	J/mol×K	805.04	Joback Method
cpg	552.44	J/mol×K	837.64	Joback Method
cpg	561.31	J/mol×K	870.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391133&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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