

Succinic acid, 2,2-dichloroethyl cis-hex-3-en-1-yl ester

Inchi: InChI=1S/C12H18Cl2O4/c1-2-3-4-5-8-17-11(15)6-7-12(16)18-9-10(13)14/h3-4,10H,2,5-9
InchiKey: HHTFMMFOZANOQM-ARJAWSKDSA-N
Formula: C12H18Cl2O4
SMILES: CCC=CCCOC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 297.18

Physical Properties

Property code	Value	Unit	Source
gf	-363.76	kJ/mol	Joback Method
hf	-700.15	kJ/mol	Joback Method
hfus	37.48	kJ/mol	Joback Method
hvap	68.96	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.013		Crippen Method
mcvol	215.000	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	1903.00		NIST Webbook
rinpol	1903.00		NIST Webbook
tb	705.12	K	Joback Method
tc	899.84	K	Joback Method
tf	409.08	K	Joback Method
vc	0.828	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.21	J/molxK	705.12	Joback Method
cpg	606.49	J/molxK	867.38	Joback Method
cpg	596.63	J/molxK	834.93	Joback Method
cpg	586.09	J/molxK	802.48	Joback Method
cpg	574.84	J/molxK	770.03	Joback Method
cpg	562.89	J/molxK	737.57	Joback Method
cpg	615.68	J/molxK	899.84	Joback Method
dvisc	0.0000986	Paxs	705.12	Joback Method

dvisc	0.0001292	Paxs	655.78	Joback Method
dvisc	0.0001769	Paxs	606.44	Joback Method
dvisc	0.0002561	Paxs	557.10	Joback Method
dvisc	0.0003985	Paxs	507.76	Joback Method
dvisc	0.0006818	Paxs	458.42	Joback Method
dvisc	0.0013278	Paxs	409.08	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U391084&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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