

Succinic acid, 2,2-dichloroethyl isobutyl ester

Inchi:	InChI=1S/C10H16Cl2O4/c1-7(2)5-15-9(13)3-4-10(14)16-6-8(11)12/h7-8H,3-6H2,1-2H3
InchiKey:	JRIJGNIUJAIFKV-UHFFFAOYSA-N
Formula:	C10H16Cl2O4
SMILES:	CC(C)COC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	271.14

Physical Properties

Property code	Value	Unit	Source
gf	-463.26	kJ/mol	Joback Method
hf	-781.37	kJ/mol	Joback Method
hfus	28.58	kJ/mol	Joback Method
hvap	64.16	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.313		Crippen Method
mvol	191.120	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook
tb	654.76	K	Joback Method
tc	849.84	K	Joback Method
tf	376.62	K	Joback Method
vc	0.730	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.82	J/molxK	654.76	Joback Method
cpg	525.89	J/molxK	817.33	Joback Method
cpg	516.21	J/molxK	784.81	Joback Method
cpg	505.86	J/molxK	752.30	Joback Method
cpg	494.84	J/molxK	719.79	Joback Method
cpg	483.16	J/molxK	687.27	Joback Method
cpg	534.91	J/molxK	849.84	Joback Method
dvisc	0.0001387	Paxs	654.76	Joback Method

dvisc	0.0001835	Paxs	608.40	Joback Method
dvisc	0.0002543	Paxs	562.05	Joback Method
dvisc	0.0003737	Paxs	515.69	Joback Method
dvisc	0.0005926	Paxs	469.33	Joback Method
dvisc	0.0010395	Paxs	422.98	Joback Method
dvisc	0.0020941	Paxs	376.62	Joback Method

Sources

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=U349404&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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