Succinic acid, 2,2-dichloroethyl 3-methylbutyl ester

Inchi: InChI=1S/C11H18Cl2O4/c1-8(2)5-6-16-10(14)3-4-11(15)17-7-9(12)13/h8-9H,3-7H2,1-2H

InchiKey: MMOQCSXVSFDWTL-UHFFFAOYSA-N

Formula: C11H18Cl2O4

SMILES: CC(C)CCOC(=O)CCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 285.16

Physical Properties

Property code	Value	Unit	Source
gf	-454.84	kJ/mol	Joback Method
hf	-802.01	kJ/mol	Joback Method
hfus	31.17	kJ/mol	Joback Method
hvap	66.39	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.703		Crippen Method
mcvol	205.210	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	1729.00		NIST Webbook
tb	677.64	K	Joback Method
tc	870.74	K	Joback Method
tf	387.89	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.77	J/mol×K	677.64	Joback Method
cpg	579.37	J/mol×K	838.56	Joback Method
cpg	569.26	J/mol×K	806.37	Joback Method
cpg	558.45	J/mol×K	774.19	Joback Method
cpg	546.93	J/mol×K	742.01	Joback Method
cpg	534.70	J/mol×K	709.82	Joback Method
cpg	588.77	J/mol×K	870.74	Joback Method
dvisc	0.0001213	Pa×s	677.64	Joback Method
dvisc	0.0001610	Pa×s	629.35	Joback Method

dvisc	0.0002241	Pa×s	581.06	Joback Method
dvisc	0.0003310	Pa×s	532.76	Joback Method
dvisc	0.0005285	Pa×s	484.47	Joback Method
dvisc	0.0009359	Pa×s	436.18	Joback Method
dvisc	0.0019110	Pa×s	387.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370960&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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