

Succinic acid, ethyl 2,2,2-trichloroethyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C8H11Cl3O4/c1-2-14-6(12)3-4-7(13)15-5-8(9,10)11/h2-5H2,1H3

KTANCHZRFSHKEZ-UHFFFAOYSA-N

C8H11Cl3O4

CCOC(=O)CCC(=O)OCC(Cl)(Cl)Cl

277.53

Physical Properties

Property code	Value	Unit	Source
gf	-484.31	kJ/mol	Joback Method
hf	-754.02	kJ/mol	Joback Method
hfus	27.23	kJ/mol	Joback Method
hvap	63.57	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.243		Crippen Method
mcvol	175.180	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpol	1564.00		NIST Webbook
rinpol	1564.00		NIST Webbook
tb	644.08	K	Joback Method
tc	851.08	K	Joback Method
tf	416.42	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.22	J/mol×K	644.08	Joback Method
cpg	443.04	J/mol×K	816.58	Joback Method
cpg	435.52	J/mol×K	782.08	Joback Method
cpg	427.39	J/mol×K	747.58	Joback Method
cpg	418.64	J/mol×K	713.08	Joback Method
cpg	409.26	J/mol×K	678.58	Joback Method
cpg	449.97	J/mol×K	851.08	Joback Method
dvisc	0.0001614	Pa×s	644.08	Joback Method

dvisc	0.0002069	Pa×s	606.14	Joback Method
dvisc	0.0002742	Pa×s	568.19	Joback Method
dvisc	0.0003782	Pa×s	530.25	Joback Method
dvisc	0.0005483	Pa×s	492.31	Joback Method
dvisc	0.0008457	Pa×s	454.36	Joback Method
dvisc	0.0014117	Pa×s	416.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349164&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

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log_{10ws}:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
rin_{pol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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