

2-[(2,2,3-Trichloropropanoyl)oxy]ethyl 2,2,3-trichloropropanoate

Inchi:	InChI=1S/C8H8Cl6O4/c9-3-7(11,12)5(15)17-1-2-18-6(16)8(13,14)4-10/h1-4H2
InchiKey:	SKXLHJXDCPXVGZ-UHFFFAOYSA-N
Formula:	C8H8Cl6O4
SMILES:	O=C(OCCOC(=O)C(Cl)(Cl)CCl)C(Cl)(Cl)CCl
Mol. weight [g/mol]:	380.87
CAS:	98546-20-4

Physical Properties

Property code	Value	Unit	Source
gf	-517.26	kJ/mol	Joback Method
hf	-809.99	kJ/mol	Joback Method
hfus	32.40	kJ/mol	Joback Method
hvap	75.43	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.898		Crippen Method
mcvol	211.900	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
tb	753.14	K	Joback Method
tc	980.64	K	Joback Method
tf	508.60	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.13	J/molxK	753.14	Joback Method
cpg	470.53	J/molxK	791.06	Joback Method
cpg	477.20	J/molxK	828.97	Joback Method
cpg	483.20	J/molxK	866.89	Joback Method
cpg	488.58	J/molxK	904.81	Joback Method
cpg	493.38	J/molxK	942.72	Joback Method
cpg	497.66	J/molxK	980.64	Joback Method
dvisc	0.0006817	Paxs	508.60	Joback Method
dvisc	0.0004207	Paxs	549.36	Joback Method

dvisc	0.0002775	Paxs	590.11	Joback Method
dvisc	0.0001932	Paxs	630.87	Joback Method
dvisc	0.0001405	Paxs	671.63	Joback Method
dvisc	0.0001060	Paxs	712.38	Joback Method
dvisc	0.0000824	Paxs	753.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C98546204&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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