

Diethylmalonic acid, di(2,2,2-trichloroethyl) ester

Inchi:	InChI=1S/C11H14Cl6O4/c1-3-9(4-2,7(18)20-5-10(12,13)14)8(19)21-6-11(15,16)17/h3-6H
InchiKey:	OAAFLQBHJGZGIM-UHFFFAOYSA-N
Formula:	C11H14Cl6O4
SMILES:	CCC(CC)(C(=O)OCC(Cl)(Cl)Cl)C(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	422.94

Physical Properties

Property code	Value	Unit	Source
gf	-489.16	kJ/mol	Joback Method
hf	-880.66	kJ/mol	Joback Method
hfus	32.76	kJ/mol	Joback Method
hvap	80.81	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.620		Crippen Method
mcvol	254.170	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinsol	1976.00		NIST Webbook
tb	818.55	K	Joback Method
tc	1046.46	K	Joback Method
tf	544.83	K	Joback Method
vc	0.961	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.08	J/molxK	818.55	Joback Method
cpg	657.27	J/molxK	1008.47	Joback Method
cpg	650.91	J/molxK	970.49	Joback Method
cpg	643.99	J/molxK	932.50	Joback Method
cpg	636.44	J/molxK	894.52	Joback Method
cpg	628.17	J/molxK	856.53	Joback Method
cpg	663.17	J/molxK	1046.46	Joback Method
dvisc	0.0000394	Paxs	818.55	Joback Method
dvisc	0.0000519	Paxs	772.93	Joback Method

dvisc	0.0000709	Paxs	727.31	Joback Method
dvisc	0.0001008	Paxs	681.69	Joback Method
dvisc	0.0001509	Paxs	636.07	Joback Method
dvisc	0.0002404	Paxs	590.45	Joback Method
dvisc	0.0004139	Paxs	544.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370471&Units=SI
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

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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