Fumaric acid, 2,4,6-trichlorophenyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C12H7Cl5O4/c13-6-3-7(14)12(8(15)4-6)21-11(19)2-1-10(18)20-5-9(16)17/h1-4

InchiKey: DGROYLRWMUMEDY-OWOJBTEDSA-N

Formula: C12H7Cl5O4

SMILES: O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCC(Cl)Cl

Mol. weight [g/mol]: 392.45

Physical Properties

Property code	Value	Unit	Source
gf	-316.03	kJ/mol	Joback Method
hf	-545.25	kJ/mol	Joback Method
hfus	42.95	kJ/mol	Joback Method
hvap	86.38	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.455		Crippen Method
mcvol	227.960	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	2398.00		NIST Webbook
rinpol	2398.00		NIST Webbook
tb	859.03	K	Joback Method
tc	1098.05	K	Joback Method
tf	562.82	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.23	J/mol×K	859.03	Joback Method
cpg	521.74	J/mol×K	898.87	Joback Method
cpg	528.43	J/mol×K	938.70	Joback Method
cpg	534.29	J/mol×K	978.54	Joback Method
cpg	539.36	J/mol×K	1018.38	Joback Method
cpg	543.65	J/mol×K	1058.22	Joback Method
cpg	547.17	J/mol×K	1098.05	Joback Method
dvisc	0.0004006	Pa×s	562.82	Joback Method

dvisc	0.0002634	Pa×s	612.19	Joback Method
dvisc	0.0001843	Pa×s	661.56	Joback Method
dvisc	0.0001356	Pa×s	710.92	Joback Method
dvisc	0.0001038	Pa×s	760.29	Joback Method
dvisc	0.0000820	Pa×s	809.66	Joback Method
dvisc	0.0000667	Pa×s	859.03	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=U405952&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