Fumaric acid, 2,2,2-trichloroethyl undecyl ester

Inchi: InChI=1S/C17H27Cl3O4/c1-2-3-4-5-6-7-8-9-10-13-23-15(21)11-12-16(22)24-14-17(18,19

InchiKey: QNUKHDVSHBDXON-VAWYXSNFSA-N

Formula: C17H27Cl3O4

SMILES: CCCCCCCCCCCOC(=O)C=CC(=O)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 401.75

Physical Properties

Property code	Value	Unit	Source
gf	-328.31	kJ/mol	Joback Method
hf	-822.56	kJ/mol	Joback Method
hfus	50.74	kJ/mol	Joback Method
hvap	83.56	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.530		Crippen Method
mcvol	297.690	ml/mol	McGowan Method
pc	1277.33	kPa	Joback Method
rinpol	2481.00		NIST Webbook
rinpol	2481.00		NIST Webbook
tb	854.16	K	Joback Method
tc	1055.49	K	Joback Method
tf	512.77	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.52	J/mol×K	854.16	Joback Method
cpg	867.30	J/mol×K	887.71	Joback Method
cpg	880.17	J/mol×K	921.27	Joback Method
cpg	892.19	J/mol×K	954.82	Joback Method
cpg	903.41	J/mol×K	988.38	Joback Method
cpg	913.86	J/mol×K	1021.93	Joback Method
cpg	923.61	J/mol×K	1055.49	Joback Method
dvisc	0.0004923	Pa×s	512.77	Joback Method

dvisc	0.0002549	Pa×s	569.67	Joback Method
dvisc	0.0001488	Pa×s	626.57	Joback Method
dvisc	0.0000950	Pa×s	683.46	Joback Method
dvisc	0.0000649	Pa×s	740.36	Joback Method
dvisc	0.0000469	Pa×s	797.26	Joback Method
dvisc	0.0000354	Pa×s	854.16	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=U348508&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