Fumaric acid, dodecyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C18H29Cl3O4/c1-2-3-4-5-6-7-8-9-10-11-14-24-16(22)12-13-17(23)25-15-18(19

InchiKey: IFPVIGYQBLXYMK-OUKQBFOZSA-N

Formula: C18H29Cl3O4

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

Mol. weight [g/mol]: 415.78

Physical Properties

Property code	Value	Unit	Source
gf	-319.89	kJ/mol	Joback Method
hf	-843.20	kJ/mol	Joback Method
hfus	53.33	kJ/mol	Joback Method
hvap	85.79	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.920		Crippen Method
mcvol	311.780	ml/mol	McGowan Method
pc	1194.00	kPa	Joback Method
rinpol	2584.00		NIST Webbook
rinpol	2584.00		NIST Webbook
tb	877.04	K	Joback Method
tc	1079.86	K	Joback Method
tf	524.04	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.61	J/mol×K	877.04	Joback Method
cpg	973.50	J/mol×K	1046.05	Joback Method
cpg	962.78	J/mol×K	1012.25	Joback Method
cpg	951.28	J/mol×K	978.45	Joback Method
cpg	938.95	J/mol×K	944.65	Joback Method
cpg	925.74	J/mol×K	910.84	Joback Method
cpg	983.50	J/mol×K	1079.86	Joback Method
dvisc	0.0000301	Pa×s	877.04	Joback Method

dvisc	0.0000400	Pa×s	818.21	Joback Method
dvisc	0.0000556	Pa×s	759.37	Joback Method
dvisc	0.0000817	Pa×s	700.54	Joback Method
dvisc	0.0001287	Pa×s	641.71	Joback Method
dvisc	0.0002222	Pa×s	582.87	Joback Method
dvisc	0.0004337	Pa×s	524.04	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=U348509&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