Fumaric acid, 2,2,2-trichloroethyl tridecyl ester

Inchi: InChI=1S/C19H31Cl3O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-25-17(23)13-14-18(24)26-16-19
InchiKey: ZTXCYTUNNUJFBB-BUHFOSPRSA-N
Formula: C19H31Cl3O4
SMILES: CCCCCCCCCCCCCOC(=O)C=CC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 429.81

Physical Properties

Property code	Value	Unit	Source
gf	-311.47	kJ/mol	Joback Method
hf	-863.84	kJ/mol	Joback Method
hfus	55.92	kJ/mol	Joback Method
hvap	88.02	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.310		Crippen Method
mcvol	325.870	ml/mol	McGowan Method
pc	1118.56	kPa	Joback Method
rinpol	2684.00		NIST Webbook
rinpol	2684.00		NIST Webbook
tb	899.92	K	Joback Method
tc	1105.02	K	Joback Method
tf	535.31	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.48	J/mol×K	899.92	Joback Method
cpg	1033.95	J/mol×K	1070.83	Joback Method
cpg	1022.96	J/mol×K	1036.65	Joback Method
cpg	1011.18	J/mol×K	1002.47	Joback Method
cpg	998.54	J/mol×K	968.29	Joback Method
cpg	984.99	J/mol×K	934.10	Joback Method
cpg	1044.20	J/mol×K	1105.02	Joback Method
dvisc	0.0000256	Pa×s	899.92	Joback Method

dvisc	0.0000341	Pa×s	839.15	Joback Method
dvisc	0.0000476	Pa×s	778.38	Joback Method
dvisc	0.0000701	Pa×s	717.62	Joback Method
dvisc	0.0001111	Pa×s	656.85	Joback Method
dvisc	0.0001932	Pa×s	596.08	Joback Method
dvisc	0.0003810	Pa×s	535.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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=U348510&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume