Fumaric acid, octyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C14H21Cl3O4/c1-2-3-4-5-6-7-10-20-12(18)8-9-13(19)21-11-14(15,16)17/h8-9H

InchiKey: ZKKSUBLUEFJBSP-CMDGGOBGSA-N

Formula: C14H21Cl3O4

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

Mol. weight [g/mol]: 359.67

Physical Properties

Property code	Value	Unit	Source
gf	-353.57	kJ/mol	Joback Method
hf	-760.64	kJ/mol	Joback Method
hfus	42.97	kJ/mol	Joback Method
hvap	76.89	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.360		Crippen Method
mcvol	255.420	ml/mol	McGowan Method
pc	1587.28	kPa	Joback Method
rinpol	2172.00		NIST Webbook
rinpol	2172.00		NIST Webbook
tb	785.52	K	Joback Method
tc	986.60	K	Joback Method
tf	478.96	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.59	J/mol×K	785.52	Joback Method
cpg	740.03	J/mol×K	953.09	Joback Method
cpg	730.43	J/mol×K	919.58	Joback Method
cpg	720.13	J/mol×K	886.06	Joback Method
cpg	709.08	J/mol×K	852.55	Joback Method
cpg	697.25	J/mol×K	819.03	Joback Method
cpg	748.95	J/mol×K	986.60	Joback Method
dvisc	0.0000567	Pa×s	785.52	Joback Method

dvisc	0.0000746	Pa×s	734.43	Joback Method
dvisc	0.0001022	Pa×s	683.33	Joback Method
dvisc	0.0001475	Pa×s	632.24	Joback Method
dvisc	0.0002268	Pa×s	581.15	Joback Method
dvisc	0.0003790	Pa×s	530.05	Joback Method
dvisc	0.0007068	Pa×s	478.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348505&Units=SI
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

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