Fumaric acid, nonyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C15H23Cl3O4/c1-2-3-4-5-6-7-8-11-21-13(19)9-10-14(20)22-12-15(16,17)18/h9
InchiKey: JRFRJYDZGXWGQR-MDZDMXLPSA-N
Formula: C15H23Cl3O4
SMILES: CCCCCCCCCOC(=O)C=CC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 373.70

Physical Properties

Property code	Value	Unit	Source
gf	-345.15	kJ/mol	Joback Method
hf	-781.28	kJ/mol	Joback Method
hfus	45.56	kJ/mol	Joback Method
hvap	79.11	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.750		Crippen Method
mcvol	269.510	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
rinpol	2276.00		NIST Webbook
rinpol	2276.00		NIST Webbook
tb	808.40	K	Joback Method
tc	1008.92	K	Joback Method
tf	490.23	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.95	J/mol×K	808.40	Joback Method
cpg	797.11	J/mol×K	975.50	Joback Method
cpg	787.21	J/mol×K	942.08	Joback Method
cpg	776.58	J/mol×K	908.66	Joback Method
cpg	765.19	J/mol×K	875.24	Joback Method
cpg	753.00	J/mol×K	841.82	Joback Method
cpg	806.32	J/mol×K	1008.92	Joback Method
dvisc	0.0000485	Pa×s	808.40	Joback Method

dvisc	0.0000640	Pa×s	755.37	Joback Method
dvisc	0.0000881	Pa×s	702.34	Joback Method
dvisc	0.0001276	Pa×s	649.31	Joback Method
dvisc	0.0001975	Pa×s	596.29	Joback Method
dvisc	0.0003330	Pa×s	543.26	Joback Method
dvisc	0.0006285	Pa×s	490.23	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=U348506&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