Fumaric acid, pentyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C11H15Cl3O4/c1-2-3-4-7-17-9(15)5-6-10(16)18-8-11(12,13)14/h5-6H,2-4,7-8H
InchiKey: CPZRBRIYEOEULK-AATRIKPKSA-N
Formula: C11H15Cl3O4
SMILES: CCCCCOC(=O)C=CC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 317.59

Physical Properties

Property code	Value	Unit	Source
gf	-378.83	kJ/mol	Joback Method
hf	-698.72	kJ/mol	Joback Method
hfus	35.20	kJ/mol	Joback Method
hvap	70.21	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.189		Crippen Method
mcvol	213.150	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
tb	716.88	K	Joback Method
tc	923.00	K	Joback Method
tf	445.15	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.05	J/mol×K	716.88	Joback Method
cpg	536.34	J/mol×K	751.23	Joback Method
cpg	546.86	J/mol×K	785.59	Joback Method
cpg	556.67	J/mol×K	819.94	Joback Method
cpg	565.78	J/mol×K	854.29	Joback Method
cpg	574.24	J/mol×K	888.65	Joback Method
cpg	582.08	J/mol×K	923.00	Joback Method
dvisc	0.0009820	Pa×s	445.15	Joback Method

dvisc	0.0005478	Pa×s	490.44	Joback Method
dvisc	0.0003373	Pa×s	535.73	Joback Method
dvisc	0.0002240	Pa×s	581.01	Joback Method
dvisc	0.0001578	Pa×s	626.30	Joback Method
dvisc	0.0001166	Pa×s	671.59	Joback Method
dvisc	0.0000895	Pa×s	716.88	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=U348504&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