Fumaric acid, 2-chlorophenyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C12H9Cl3O4/c13-8-3-1-2-4-9(8)19-12(17)6-5-11(16)18-7-10(14)15/h1-6,10H,7

InchiKey: WYSRASHEXLSRMZ-AATRIKPKSA-N

Formula: C12H9Cl3O4

SMILES: O=C(C=CC(=O)Oc1ccccc1Cl)OCC(Cl)Cl

Mol. weight [g/mol]: 323.56

Physical Properties

Property code	Value	Unit	Source
gf	-272.91	kJ/mol	Joback Method
hf	-490.83	kJ/mol	Joback Method
hfus	35.33	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.149		Crippen Method
mcvol	203.480	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	2139.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	774.21	K	Joback Method
tc	1006.92	K	Joback Method
tf	477.94	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.43	J/mol×K	774.21	Joback Method
cpg	491.22	J/mol×K	813.00	Joback Method
cpg	500.14	J/mol×K	851.78	Joback Method
cpg	508.21	J/mol×K	890.57	Joback Method
cpg	515.47	J/mol×K	929.35	Joback Method
cpg	521.93	J/mol×K	968.14	Joback Method
cpg	527.62	J/mol×K	1006.92	Joback Method
dvisc	0.0007508	Pa×s	477.94	Joback Method

dvisc	0.0004435	Pa×s	527.32	Joback Method
dvisc	0.0002867	Pa×s	576.70	Joback Method
dvisc	0.0001985	Pa×s	626.08	Joback Method
dvisc	0.0001451	Pa×s	675.45	Joback Method
dvisc	0.0001106	Pa×s	724.83	Joback Method
dvisc	0.0000873	Pa×s	774.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405722&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