Fumaric acid, 2,4-dichlorophenyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C12H8Cl4O4/c13-7-1-2-9(8(14)5-7)20-12(18)4-3-11(17)19-6-10(15)16/h1-5,10

InchiKey: ROOBKPXDNAQUAD-ONEGZZNKSA-N

Formula: C12H8Cl4O4

SMILES: O=C(C=CC(=O)Oc1ccc(Cl)cc1Cl)OCC(Cl)Cl

Mol. weight [g/mol]: 358.00

Physical Properties

Property code	Value	Unit	Source
gf	-294.47	kJ/mol	Joback Method
hf	-518.04	kJ/mol	Joback Method
hfus	39.14	kJ/mol	Joback Method
hvap	81.33	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.802		Crippen Method
mcvol	215.720	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	2307.00		NIST Webbook
rinpol	2307.00		NIST Webbook
tb	816.62	K	Joback Method
tc	1052.51	K	Joback Method
tf	520.38	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.69	J/mol×K	816.62	Joback Method
cpg	507.33	J/mol×K	855.93	Joback Method
cpg	515.11	J/mol×K	895.25	Joback Method
cpg	522.08	J/mol×K	934.56	Joback Method
cpg	528.23	J/mol×K	973.88	Joback Method
cpg	533.61	J/mol×K	1013.19	Joback Method
cpg	538.23	J/mol×K	1052.51	Joback Method
dvisc	0.0005416	Pa×s	520.38	Joback Method

dvisc	0.0003393	Pa×s	569.75	Joback Method
dvisc	0.0002291	Pa×s	619.13	Joback Method
dvisc	0.0001639	Pa×s	668.50	Joback Method
dvisc	0.0001228	Pa×s	717.87	Joback Method
dvisc	0.0000955	Pa×s	767.25	Joback Method
dvisc	0.0000765	Pa×s	816.62	Joback Method

Sources

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=U405695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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