Fumaric acid, 2,5-dichlorophenyl 3-chlorophenyl ester

Inchi: InChI=1S/C16H9Cl3O4/c17-10-2-1-3-12(8-10)22-15(20)6-7-16(21)23-14-9-11(18)4-5-13(

InchiKey: XEPNHJDMYDWNFZ-VOTSOKGWSA-N

Formula: C16H9Cl3O4

SMILES: O=C(C=CC(=O)Oc1cc(Cl)ccc1Cl)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 371.60

Physical Properties

Property code	Value	Unit	Source
gf	-143.64	kJ/mol	Joback Method
hf	-354.52	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	89.17	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.714		Crippen Method
mcvol	236.080	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	2639.00		NIST Webbook
rinpol	2639.00		NIST Webbook
tb	902.81	K	Joback Method
tc	1154.56	K	Joback Method
tf	589.48	K	Joback Method
vc	0.890	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.02	J/mol×K	902.81	Joback Method
cpg	622.99	J/mol×K	1112.60	Joback Method
cpg	618.16	J/mol×K	1070.65	Joback Method
cpg	612.39	J/mol×K	1028.69	Joback Method
cpg	605.64	J/mol×K	986.73	Joback Method
cpg	597.86	J/mol×K	944.77	Joback Method
cpg	626.94	J/mol×K	1154.56	Joback Method
dvisc	0.0000577	Pa×s	902.81	Joback Method

dvisc	0.0000705	Pa×s	850.59	Joback Method
dvisc	0.0000885	Pa×s	798.37	Joback Method
dvisc	0.0001147	Pa×s	746.14	Joback Method
dvisc	0.0001545	Pa×s	693.92	Joback Method
dvisc	0.0002186	Pa×s	641.70	Joback Method
dvisc	0.0003288	Pa×s	589.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405972&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