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

Inchi: InChI=1S/C18H14Cl2O4/c1-11-8-12(2)10-13(9-11)23-16(21)6-7-17(22)24-15-5-3-4-14(19

InchiKey: QCNMVAZLWTYELH-VOTSOKGWSA-N

Formula: C18H14Cl2O4

SMILES: Cc1cc(C)cc(OC(=O)C=CC(=O)Oc2cccc(Cl)c2Cl)c1

Mol. weight [g/mol]: 365.21

Physical Properties

Property code	Value	Unit	Source
gf	-124.50	kJ/mol	Joback Method
hf	-391.53	kJ/mol	Joback Method
hfus	43.07	kJ/mol	Joback Method
hvap	89.90	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.677		Crippen Method
mcvol	252.020	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	2746.00		NIST Webbook
rinpol	2746.00		NIST Webbook
tb	916.12	K	Joback Method
tc	1159.25	K	Joback Method
tf	594.62	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.20	J/mol×K	916.12	Joback Method
cpg	720.77	J/mol×K	1118.73	Joback Method
cpg	714.61	J/mol×K	1078.21	Joback Method
cpg	707.41	J/mol×K	1037.68	Joback Method
cpg	699.13	J/mol×K	997.16	Joback Method
cpg	689.74	J/mol×K	956.64	Joback Method
cpg	725.92	J/mol×K	1159.25	Joback Method
dvisc	0.0000515	Pa×s	916.12	Joback Method

dvisc	0.0000628	Pa×s	862.54	Joback Method
dvisc	0.0000786	Pa×s	808.95	Joback Method
dvisc	0.0001016	Pa×s	755.37	Joback Method
dvisc	0.0001365	Pa×s	701.79	Joback Method
dvisc	0.0001926	Pa×s	648.20	Joback Method
dvisc	0.0002892	Pa×s	594.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405743&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