Fumaric acid, 2,4,6-trichlorophenyl dec-2-yl ester

Inchi: InChI=1S/C20H25Cl3O4/c1-3-4-5-6-7-8-9-14(2)26-18(24)10-11-19(25)27-20-16(22)12-15

InchiKey: GXRQJDLLNGSBBD-ZHACJKMWSA-N

Formula: C20H25Cl3O4

SMILES: CCCCCCCCC(C)OC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 435.77

Physical Properties

Property code	Value	Unit	Source
gf	-224.81	kJ/mol	Joback Method
hf	-678.89	kJ/mol	Joback Method
hfus	55.27	kJ/mol	Joback Method
hvap	95.41	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.791		Crippen Method
mcvol	316.200	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	2783.00		NIST Webbook
rinpol	2783.00		NIST Webbook
tb	967.21	K	Joback Method
tc	1190.31	K	Joback Method
tf	593.14	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.51	J/mol×K	967.21	Joback Method
cpg	934.69	J/mol×K	1004.39	Joback Method
cpg	945.73	J/mol×K	1041.58	Joback Method
cpg	955.67	J/mol×K	1078.76	Joback Method
cpg	964.56	J/mol×K	1115.94	Joback Method
cpg	972.43	J/mol×K	1153.13	Joback Method
cpg	979.32	J/mol×K	1190.31	Joback Method
dvisc	0.0002497	Pa×s	593.14	Joback Method

dvisc	0.0001462	Pa×s	655.49	Joback Method
dvisc	0.0000939	Pa×s	717.83	Joback Method
dvisc	0.0000648	Pa×s	780.17	Joback Method
dvisc	0.0000472	Pa×s	842.52	Joback Method
dvisc	0.0000359	Pa×s	904.87	Joback Method
dvisc	0.0000283	Pa×s	967.21	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=U405958&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