Fumaric acid, 2,4,4-trimethylpentyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C18H22Cl2O4/c1-12(10-18(2,3)4)11-23-15(21)8-9-16(22)24-14-7-5-6-13(19)17

InchiKey: VQXNOVCJKSDXFJ-CMDGGOBGSA-N

Formula: C18H22Cl2O4

SMILES: CC(COC(=O)C=CC(=O)Oc1cccc(Cl)c1Cl)CC(C)(C)C

Mol. weight [g/mol]: 373.27

Physical Properties

Property code	Value	Unit	Source
gf	-217.25	kJ/mol	Joback Method
hf	-619.15	kJ/mol	Joback Method
hfus	38.87	kJ/mol	Joback Method
hvap	84.62	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	5.071		Crippen Method
mcvol	275.780	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	2471.00		NIST Webbook
rinpol	2471.00		NIST Webbook
tb	875.81	K	Joback Method
tc	1099.10	K	Joback Method
tf	530.58	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.54	J/mol×K	875.81	Joback Method
cpg	799.66	J/mol×K	913.03	Joback Method
cpg	811.75	J/mol×K	950.24	Joback Method
cpg	822.84	J/mol×K	987.46	Joback Method
cpg	833.00	J/mol×K	1024.67	Joback Method
cpg	842.28	J/mol×K	1061.89	Joback Method
cpg	850.75	J/mol×K	1099.10	Joback Method
dvisc	0.0003895	Pa×s	530.58	Joback Method

dvisc	0.0002131	Pa×s	588.12	Joback Method
dvisc	0.0001299	Pa×s	645.66	Joback Method
dvisc	0.0000858	Pa×s	703.19	Joback Method
dvisc	0.0000604	Pa×s	760.73	Joback Method
dvisc	0.0000446	Pa×s	818.27	Joback Method
dvisc	0.0000343	Pa×s	875.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405611&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