Fumaric acid, 2,4,4-trimethylpentyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C18H21Cl3O4/c1-11(9-18(2,3)4)10-24-15(22)5-6-16(23)25-17-13(20)7-12(19)8

InchiKey: GONFSCGHIVWZIX-AATRIKPKSA-N

Formula: C18H21Cl3O4

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

Mol. weight [g/mol]: 407.72

Physical Properties

Property code	Value	Unit	Source
gf	-238.81	kJ/mol	Joback Method
hf	-646.36	kJ/mol	Joback Method
hfus	42.68	kJ/mol	Joback Method
hvap	89.66	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	5.724		Crippen Method
mcvol	288.020	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook
tb	918.22	K	Joback Method
tc	1145.98	K	Joback Method
tf	573.02	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.23	J/mol×K	918.22	Joback Method
cpg	819.12	J/mol×K	956.18	Joback Method
cpg	830.00	J/mol×K	994.14	Joback Method
cpg	839.92	J/mol×K	1032.10	Joback Method
cpg	848.93	J/mol×K	1070.06	Joback Method
cpg	857.10	J/mol×K	1108.02	Joback Method
cpg	864.47	J/mol×K	1145.98	Joback Method
dvisc	0.0002721	Pa×s	573.02	Joback Method

dvisc	0.0001586	Pa×s	630.55	Joback Method
dvisc	0.0001012	Pa×s	688.09	Joback Method
dvisc	0.0000692	Pa×s	745.62	Joback Method
dvisc	0.0000500	Pa×s	803.15	Joback Method
dvisc	0.0000377	Pa×s	860.69	Joback Method
dvisc	0.0000294	Pa×s	918.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405613&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