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

Inchi: InChI=1S/C18H13Cl3O4/c19-13-10-14(20)18(15(21)11-13)25-17(23)7-6-16(22)24-9-8-12

InchiKey: KEKSIWZMPRYBRX-VOTSOKGWSA-N

Formula: C18H13Cl3O4

SMILES: O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCCc1ccccc1

Mol. weight [g/mol]: 399.65

Physical Properties

Property code	Value	Unit	Source
gf	-126.80	kJ/mol	Joback Method
hf	-395.80	kJ/mol	Joback Method
hfus	47.66	kJ/mol	Joback Method
hvap	93.62	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	4.894		Crippen Method
mcvol	264.260	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	2788.00		NIST Webbook
rinpol	2788.00		NIST Webbook
tb	948.57	K	Joback Method
tc	1193.72	K	Joback Method
tf	612.02	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.44	J/mol×K	948.57	Joback Method
cpg	708.82	J/mol×K	989.43	Joback Method
cpg	717.10	J/mol×K	1030.29	Joback Method
cpg	724.34	J/mol×K	1071.14	Joback Method
cpg	730.58	J/mol×K	1112.00	Joback Method
cpg	735.88	J/mol×K	1152.86	Joback Method
cpg	740.30	J/mol×K	1193.72	Joback Method
dvisc	0.0002686	Pa×s	612.02	Joback Method

dvisc	0.0001744	Pa×s	668.11	Joback Method
dvisc	0.0001211	Pa×s	724.20	Joback Method
dvisc	0.0000887	Pa×s	780.29	Joback Method
dvisc	0.0000677	Pa×s	836.39	Joback Method
dvisc	0.0000534	Pa×s	892.48	Joback Method
dvisc	0.0000434	Pa×s	948.57	Joback Method

Sources

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=U405685&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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