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

Inchi: InChI=1S/C18H21Cl3O4/c1-3-4-5-6-7-12(2)24-16(22)8-9-17(23)25-18-14(20)10-13(19)11

InchiKey: YICOYUMTYGGFAX-CMDGGOBGSA-N

Formula: C18H21Cl3O4

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

Mol. weight [g/mol]: 407.72

Physical Properties

Property code	Value	Unit	Source
gf	-241.65	kJ/mol	Joback Method
hf	-637.61	kJ/mol	Joback Method
hfus	50.09	kJ/mol	Joback Method
hvap	90.96	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	6.010		Crippen Method
mcvol	288.020	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	2576.00		NIST Webbook
rinpol	2576.00		NIST Webbook
tb	921.45	K	Joback Method
tc	1142.93	K	Joback Method
tf	570.60	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.41	J/mol×K	921.45	Joback Method
cpg	818.15	J/mol×K	958.36	Joback Method
cpg	828.83	J/mol×K	995.28	Joback Method
cpg	838.49	J/mol×K	1032.19	Joback Method
cpg	847.16	J/mol×K	1069.10	Joback Method
cpg	854.86	J/mol×K	1106.02	Joback Method
cpg	861.63	J/mol×K	1142.93	Joback Method
dvisc	0.0003122	Pa×s	570.60	Joback Method

dvisc	0.0001869	Pa×s	629.08	Joback Method
dvisc	0.0001221	Pa×s	687.55	Joback Method
dvisc	0.0000853	Pa×s	746.02	Joback Method
dvisc	0.0000627	Pa×s	804.50	Joback Method
dvisc	0.0000481	Pa×s	862.97	Joback Method
dvisc	0.0000382	Pa×s	921.45	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=U405593&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