Fumaric acid, octyl 2,3,6-trichlorophenyl ester

Inchi: InChI=1S/C18H21Cl3O4/c1-2-3-4-5-6-7-12-24-15(22)10-11-16(23)25-18-14(20)9-8-13(19
InchiKey: IRUIEEPNBKTVAT-ZHACJKMWSA-N
Formula: C18H21Cl3O4
SMILES: CCCCCCCCOC(=O)C=CC(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 407.72

Physical Properties

Property code	Value	Unit	Source
gf	-239.21	kJ/mol	Joback Method
hf	-632.33	kJ/mol	Joback Method
hfus	53.62	kJ/mol	Joback Method
hvap	91.35	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	6.012		Crippen Method
mcvol	288.020	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	2785.00		NIST Webbook
tb	921.89	K	Joback Method
tc	1141.42	K	Joback Method
tf	585.60	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.90	J/mol×K	921.89	Joback Method
cpg	817.57	J/mol×K	958.48	Joback Method
cpg	828.23	J/mol×K	995.07	Joback Method
cpg	837.89	J/mol×K	1031.66	Joback Method
cpg	846.58	J/mol×K	1068.25	Joback Method
cpg	854.35	J/mol×K	1104.83	Joback Method
cpg	861.21	J/mol×K	1141.42	Joback Method
dvisc	0.0002906	Pa×s	585.60	Joback Method
dvisc	0.0001827	Pa×s	641.65	Joback Method

dvisc	0.0001237	Pa×s	697.70	Joback Method
dvisc	0.0000888	Pa×s	753.75	Joback Method
dvisc	0.0000667	Pa×s	809.79	Joback Method
dvisc	0.0000520	Pa×s	865.84	Joback Method
dvisc	0.0000418	Pa×s	921.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348227&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