Fumaric acid, octyl 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C18H20Cl4O4/c1-2-3-4-5-6-7-10-25-14(23)8-9-15(24)26-18-13(20)11-12(19)16
InchiKey: FBMUHQGBYTWMGK-CMDGGOBGSA-N
Formula: C18H20Cl4O4
SMILES: CCCCCCCCOC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 442.16

Physical Properties

Property code	Value	Unit	Source
gf	-260.77	kJ/mol	Joback Method
hf	-659.54	kJ/mol	Joback Method
hfus	57.42	kJ/mol	Joback Method
hvap	96.40	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.665		Crippen Method
mcvol	300.260	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpol	2928.00		NIST Webbook
tb	964.30	K	Joback Method
tc	1189.66	K	Joback Method
tf	628.04	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.82	J/mol×K	964.30	Joback Method
cpg	867.11	J/mol×K	1152.10	Joback Method
cpg	860.63	J/mol×K	1114.54	Joback Method
cpg	853.19	J/mol×K	1076.98	Joback Method
cpg	844.76	J/mol×K	1039.42	Joback Method
cpg	835.31	J/mol×K	1001.86	Joback Method
cpg	872.65	J/mol×K	1189.66	Joback Method
dvisc	0.0000363	Pa×s	964.30	Joback Method
dvisc	0.0000446	Pa×s	908.26	Joback Method

dvisc	0.0000563	Pa×s	852.21	Joback Method
dvisc	0.0000736	Pa×s	796.17	Joback Method
dvisc	0.0001001	Pa×s	740.13	Joback Method
dvisc	0.0001431	Pa×s	684.08	Joback Method
dvisc	0.0002181	Pa×s	628.04	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=U348200&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

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