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

Inchi: InChI=1S/C21H26Cl4O4/c1-2-3-4-5-6-7-8-9-10-13-28-17(26)11-12-18(27)29-21-16(23)14
InchiKey: BAXHBOKGWTUNMQ-VAWYXSNFSA-N
Formula: C21H26Cl4O4
SMILES: CCCCCCCCCCCOC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 484.24

Physical Properties

Property code	Value	Unit	Source
gf	-235.51	kJ/mol	Joback Method
hf	-721.46	kJ/mol	Joback Method
hfus	65.20	kJ/mol	Joback Method
hvap	103.07	kJ/mol	Joback Method
log10ws	-8.68		Crippen Method
logp	7.836		Crippen Method
mcvol	342.530	ml/mol	McGowan Method
pc	1135.96	kPa	Joback Method
rinpol	3253.00		NIST Webbook
tb	1032.94	K	Joback Method
tc	1265.38	K	Joback Method
tf	661.85	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.08	J/mol×K	1032.94	Joback Method
cpg	1011.27	J/mol×K	1071.68	Joback Method
cpg	1021.25	J/mol×K	1110.42	Joback Method
cpg	1030.08	J/mol×K	1149.16	Joback Method
cpg	1037.78	J/mol×K	1187.90	Joback Method
cpg	1044.41	J/mol×K	1226.64	Joback Method
cpg	1050.00	J/mol×K	1265.38	Joback Method
dvisc	0.0001549	Pa×s	661.85	Joback Method
dvisc	0.0000984	Pa×s	723.70	Joback Method

dvisc	0.0000671	Pa×s	785.55	Joback Method
dvisc	0.0000484	Pa×s	847.39	Joback Method
dvisc	0.0000365	Pa×s	909.24	Joback Method
dvisc	0.0000286	Pa×s	971.09	Joback Method
dvisc	0.0000230	Pa×s	1032.94	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U348203&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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