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

Inchi: InChI=1S/C19H22Cl4O4/c1-2-3-4-5-6-7-8-11-26-15(24)9-10-16(25)27-19-14(21)12-13(20

InchiKey: HXFNNNWNGSGHRR-MDZDMXLPSA-N

Formula: C19H22Cl4O4

SMILES: CCCCCCCCCOC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 456.19

Physical Properties

Property code	Value	Unit	Source
gf	-252.35	kJ/mol	Joback Method
hf	-680.18	kJ/mol	Joback Method
hfus	60.01	kJ/mol	Joback Method
hvap	98.62	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	7.056		Crippen Method
mcvol	314.350	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	3044.00		NIST Webbook
tb	987.18	K	Joback Method
tc	1213.95	K	Joback Method
tf	639.31	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.64	J/mol×K	987.18	Joback Method
cpg	925.69	J/mol×K	1176.16	Joback Method
cpg	919.14	J/mol×K	1138.36	Joback Method
cpg	911.59	J/mol×K	1100.57	Joback Method
cpg	903.01	J/mol×K	1062.77	Joback Method
cpg	893.37	J/mol×K	1024.98	Joback Method
cpg	931.28	J/mol×K	1213.95	Joback Method
dvisc	0.0000312	Pa×s	987.18	Joback Method
dvisc	0.0000385	Pa×s	929.20	Joback Method

dvisc	0.0000489	Pa×s	871.22	Joback Method
dvisc	0.0000641	Pa×s	813.25	Joback Method
dvisc	0.0000878	Pa×s	755.27	Joback Method
dvisc	0.0001266	Pa×s	697.29	Joback Method
dvisc	0.0001952	Pa×s	639.31	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348201&Units=SI

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