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

Inchi: InChI=1S/C20H24Cl4O4/c1-2-3-4-5-6-7-8-9-12-27-16(25)10-11-17(26)28-20-15(22)13-14

InchiKey: XGVVNHSYZDSMHW-ZHACJKMWSA-N

Formula: C20H24Cl4O4

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

Mol. weight [g/mol]: 470.21

Physical Properties

Property code	Value	Unit	Source
gf	-243.93	kJ/mol	Joback Method
hf	-700.82	kJ/mol	Joback Method
hfus	62.60	kJ/mol	Joback Method
hvap	100.85	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.446		Crippen Method
mcvol	328.440	ml/mol	McGowan Method
pc	1213.20	kPa	Joback Method
rinpol	3149.00		NIST Webbook
tb	1010.06	K	Joback Method
tc	1239.17	K	Joback Method
tf	650.58	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.08	J/mol×K	1010.06	Joback Method
cpg	952.04	J/mol×K	1048.25	Joback Method
cpg	961.86	J/mol×K	1086.43	Joback Method
cpg	970.57	J/mol×K	1124.62	Joback Method
cpg	978.20	J/mol×K	1162.80	Joback Method
cpg	984.81	J/mol×K	1200.99	Joback Method
cpg	990.41	J/mol×K	1239.17	Joback Method
dvisc	0.0001741	Pa×s	650.58	Joback Method
dvisc	0.0001118	Pa×s	710.49	Joback Method

dvisc	0.0000769	Pa×s	770.41	Joback Method
dvisc	0.0000558	Pa×s	830.32	Joback Method
dvisc	0.0000423	Pa×s	890.23	Joback Method
dvisc	0.0000332	Pa×s	950.15	Joback Method
dvisc	0.0000268	Pa×s	1010.06	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=U348202&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