Phthalic acid, decyl 3,4,5-trichlorophenyl ester

Inchi: InChI=1S/C24H27Cl3O4/c1-2-3-4-5-6-7-8-11-14-30-23(28)18-12-9-10-13-19(18)24(29)31
InchiKey: UHCQTCFFSZGMOQ-UHFFFAOYSA-N
Formula: C24H27Cl3O4
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]: 485.83

Physical Properties

Property code	Value	Unit	Source
gf	-166.13	kJ/mol	Joback Method
hf	-648.33	kJ/mol	Joback Method
hfus	62.61	kJ/mol	Joback Method
hvap	107.68	kJ/mol	Joback Method
log10ws	-9.62		Crippen Method
logp	8.163		Crippen Method
mcvol	353.100	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	3387.00		NIST Webbook
rinpol	3387.00		NIST Webbook
tb	1086.67	K	Joback Method
tc	1331.19	K	Joback Method
tf	697.24	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.42	J/mol×K	1086.67	Joback Method
cpg	1084.30	J/mol×K	1127.42	Joback Method
cpg	1092.67	J/mol×K	1168.18	Joback Method
cpg	1099.58	J/mol×K	1208.93	Joback Method
cpg	1105.09	J/mol×K	1249.68	Joback Method
cpg	1109.23	J/mol×K	1290.44	Joback Method
cpg	1112.07	J/mol×K	1331.19	Joback Method
dvisc	0.0001366	Pa×s	697.24	Joback Method

dvisc	0.0000871	Pa×s	762.14	Joback Method
dvisc	0.0000596	Pa×s	827.05	Joback Method
dvisc	0.0000431	Pa×s	891.96	Joback Method
dvisc	0.0000326	Pa×s	956.86	Joback Method
dvisc	0.0000255	Pa×s	1021.77	Joback Method
dvisc	0.0000206	Pa×s	1086.67	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=U357073&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