Phthalic acid, dodecyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C26H31Cl3O4/c1-2-3-4-5-6-7-8-9-10-13-16-32-25(30)19-14-11-12-15-20(19)26

InchiKey: CDQHZKJZRJBGJC-UHFFFAOYSA-N

Formula: C26H31Cl3O4

SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 513.88

Physical Properties

Property code	Value	Unit	Source
gf	-149.29	kJ/mol	Joback Method
hf	-689.61	kJ/mol	Joback Method
hfus	67.79	kJ/mol	Joback Method
hvap	112.14	kJ/mol	Joback Method
log10ws	-10.46		Crippen Method
logp	8.944		Crippen Method
mcvol	381.280	ml/mol	McGowan Method
pc	1020.08	kPa	Joback Method
rinpol	3534.00		NIST Webbook
tb	1132.43	K	Joback Method
tc	1386.83	K	Joback Method
tf	719.78	K	Joback Method
vc	1.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1193.79	J/mol×K	1132.43	Joback Method
cpg	1203.72	J/mol×K	1174.83	Joback Method
cpg	1211.99	J/mol×K	1217.23	Joback Method
cpg	1218.67	J/mol×K	1259.63	Joback Method
cpg	1223.83	J/mol×K	1302.03	Joback Method
cpg	1227.52	J/mol×K	1344.43	Joback Method
cpg	1229.83	J/mol×K	1386.83	Joback Method
dvisc	0.0001069	Pa×s	719.78	Joback Method
dvisc	0.0000668	Pa×s	788.55	Joback Method

dvisc	0.0000451	Pa×s	857.33	Joback Method
dvisc	0.0000322	Pa×s	926.11	Joback Method
dvisc	0.0000242	Pa×s	994.88	Joback Method
dvisc	0.0000188	Pa×s	1063.66	Joback Method
dvisc	0.0000151	Pa×s	1132.43	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=U357052&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