

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)2
InchiKey:	CDQHZKJZRJBGJC-UHFFFAOYSA-N
Formula:	C26H31Cl3O4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc1C(=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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000451	Paxs	857.33	Joback Method
dvisc	0.0000322	Paxs	926.11	Joback Method
dvisc	0.0000242	Paxs	994.88	Joback Method
dvisc	0.0000188	Paxs	1063.66	Joback Method
dvisc	0.0000151	Paxs	1132.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357052&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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