

Phthalic acid, 4-chloro-2-methylphenyl dodecyl ester

Inchi:	InChI=1S/C27H35ClO4/c1-3-4-5-6-7-8-9-10-11-14-19-31-26(29)23-15-12-13-16-24(23)27
InchiKey:	BUABLNGWBIWGDH-UHFFFAOYSA-N
Formula:	C27H35ClO4
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1ccc(Cl)cc1C
Mol. weight [g/mol]:	459.02

Physical Properties

Property code	Value	Unit	Source
gf	-107.38	kJ/mol	Joback Method
hf	-667.30	kJ/mol	Joback Method
hfus	62.37	kJ/mol	Joback Method
hvap	104.93	kJ/mol	Joback Method
log10ws	-9.57		Crippen Method
logp	7.945		Crippen Method
mcvol	370.890	ml/mol	McGowan Method
pc	1015.53	kPa	Joback Method
rinpol	3333.00		NIST Webbook
rinpol	3333.00		NIST Webbook
tb	1075.47	K	Joback Method
tc	1316.69	K	Joback Method
tf	658.69	K	Joback Method
vc	1.429	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.40	J/molxK	1075.47	Joback Method
cpg	1231.36	J/molxK	1115.67	Joback Method
cpg	1242.68	J/molxK	1155.88	Joback Method
cpg	1252.44	J/molxK	1196.08	Joback Method
cpg	1260.69	J/molxK	1236.28	Joback Method
cpg	1267.50	J/molxK	1276.48	Joback Method
cpg	1272.94	J/molxK	1316.69	Joback Method
dvisc	0.0001565	Paxs	658.69	Joback Method

dvisc	0.0000919	Paxs	728.15	Joback Method
dvisc	0.0000592	Paxs	797.62	Joback Method
dvisc	0.0000410	Paxs	867.08	Joback Method
dvisc	0.0000299	Paxs	936.54	Joback Method
dvisc	0.0000228	Paxs	1006.01	Joback Method
dvisc	0.0000180	Paxs	1075.47	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=U356382&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

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