

Phthalic acid, 2-(4-chlorophenyl)ethyl dodecyl ester

Inchi:	InChI=1S/C28H37ClO4/c1-2-3-4-5-6-7-8-9-10-13-21-32-27(30)25-14-11-12-15-26(25)28
InchiKey:	UDQPOWPWTFZRBA-UHFFFAOYSA-N
Formula:	C28H37ClO4
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1ccc(Cl)cc1
Mol. weight [g/mol]:	473.04

Physical Properties

Property code	Value	Unit	Source
gf	-89.33	kJ/mol	Joback Method
hf	-676.47	kJ/mol	Joback Method
hfus	65.35	kJ/mol	Joback Method
hvap	106.50	kJ/mol	Joback Method
log10ws	-9.28		Crippen Method
logp	7.817		Crippen Method
mvol	384.980	ml/mol	McGowan Method
pc	965.07	kPa	Joback Method
rinpol	3506.00		NIST Webbook
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tb	1093.37	K	Joback Method
tc	1339.26	K	Joback Method
tf	657.44	K	Joback Method
vc	1.484	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1280.99	J/molxK	1093.37	Joback Method
cpg	1331.80	J/molxK	1298.28	Joback Method
cpg	1324.61	J/molxK	1257.30	Joback Method
cpg	1316.02	J/molxK	1216.32	Joback Method
cpg	1305.94	J/molxK	1175.33	Joback Method
cpg	1294.29	J/molxK	1134.35	Joback Method
cpg	1337.67	J/molxK	1339.26	Joback Method
dvisc	0.0000150	Paxs	1093.37	Joback Method

dvisc	0.0000192	Paxs	1020.71	Joback Method
dvisc	0.0000256	Paxs	948.06	Joback Method
dvisc	0.0000357	Paxs	875.40	Joback Method
dvisc	0.0000530	Paxs	802.75	Joback Method
dvisc	0.0000851	Paxs	730.10	Joback Method
dvisc	0.0001517	Paxs	657.44	Joback Method

Sources

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=U377846&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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