

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

Inchi:	InChI=1S/C24H29ClO4/c1-2-3-4-5-6-9-17-28-23(26)21-10-7-8-11-22(21)24(27)29-18-16
InchiKey:	IWKJRJMQAVVRJZ-UHFFFAOYSA-N
Formula:	C24H29ClO4
SMILES:	CCCCCCCCOC(=O)c1cccc1C(=O)OCCc1ccc(Cl)cc1
Mol. weight [g/mol]:	416.94

Physical Properties

Property code	Value	Unit	Source
gf	-123.01	kJ/mol	Joback Method
hf	-593.91	kJ/mol	Joback Method
hfus	54.99	kJ/mol	Joback Method
hvap	97.59	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	6.257		Crippen Method
mvol	328.620	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	3099.00		NIST Webbook
rinpol	3099.00		NIST Webbook
tb	1001.85	K	Joback Method
tc	1231.17	K	Joback Method
tf	612.36	K	Joback Method
vc	1.260	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.35	J/molxK	1001.85	Joback Method
cpg	1051.32	J/molxK	1040.07	Joback Method
cpg	1062.88	J/molxK	1078.29	Joback Method
cpg	1073.08	J/molxK	1116.51	Joback Method
cpg	1081.98	J/molxK	1154.73	Joback Method
cpg	1089.64	J/molxK	1192.95	Joback Method
cpg	1096.10	J/molxK	1231.17	Joback Method
dvisc	0.0002457	Paxs	612.36	Joback Method

dvisc	0.0001434	Paxs	677.27	Joback Method
dvisc	0.0000919	Paxs	742.19	Joback Method
dvisc	0.0000633	Paxs	807.11	Joback Method
dvisc	0.0000461	Paxs	872.02	Joback Method
dvisc	0.0000350	Paxs	936.93	Joback Method
dvisc	0.0000276	Paxs	1001.85	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=U377842&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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