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

Inchi: InChI=1S/C21H23ClO4/c1-3-4-5-8-13-25-20(23)17-9-6-7-10-18(17)21(24)26-19-12-11-16

InchiKey: KMLUVXPBRUGZOL-UHFFFAOYSA-N

Formula: C21H23ClO4

SMILES: CCCCCCOC(=O)c1ccccc1C(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 374.86

Physical Properties

Property code	Value	Unit	Source
gf	-157.90	kJ/mol	Joback Method
hf	-543.46	kJ/mol	Joback Method
hfus	46.83	kJ/mol	Joback Method
hvap	91.58	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	5.605		Crippen Method
mcvol	286.350	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2711.00		NIST Webbook
tb	938.19	K	Joback Method
tc	1166.13	K	Joback Method
tf	591.07	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.94	J/mol×K	938.19	Joback Method
cpg	910.35	J/mol×K	1128.14	Joback Method
cpg	902.79	J/mol×K	1090.15	Joback Method
cpg	894.00	J/mol×K	1052.16	Joback Method
cpg	883.95	J/mol×K	1014.17	Joback Method
cpg	872.61	J/mol×K	976.18	Joback Method
cpg	916.71	J/mol×K	1166.13	Joback Method
dvisc	0.0000438	Pa×s	938.19	Joback Method
dvisc	0.0000545	Pa×s	880.34	Joback Method

dvisc	0.0000699	Pa×s	822.48	Joback Method
dvisc	0.0000930	Pa×s	764.63	Joback Method
dvisc	0.0001297	Pa×s	706.78	Joback Method
dvisc	0.0001920	Pa×s	648.92	Joback Method
dvisc	0.0003069	Pa×s	591.07	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=U356654&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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