

Isophthalic acid, 4-chloro-3-methylphenyl hexyl ester

Inchi:	InChI=1S/C21H23ClO4/c1-3-4-5-6-12-25-20(23)16-8-7-9-17(14-16)21(24)26-18-10-11-19
InchiKey:	RCPYFJCPLQOTIO-UHFFFAOYSA-N
Formula:	C21H23ClO4
SMILES:	CCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)c(C)c2)c1
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	3014.00		NIST Webbook
rinpol	3014.00		NIST Webbook
tb	938.19	K	Joback Method
tc	1166.13	K	Joback Method
tf	591.07	K	Joback Method
vc	1.093	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.94	J/molxK	938.19	Joback Method
cpg	910.35	J/molxK	1128.14	Joback Method
cpg	902.79	J/molxK	1090.15	Joback Method
cpg	894.00	J/molxK	1052.16	Joback Method
cpg	883.95	J/molxK	1014.17	Joback Method
cpg	872.61	J/molxK	976.18	Joback Method
cpg	916.71	J/molxK	1166.13	Joback Method
dvisc	0.0000438	Paxs	938.19	Joback Method

dvisc	0.0000545	Paxs	880.34	Joback Method
dvisc	0.0000699	Paxs	822.48	Joback Method
dvisc	0.0000930	Paxs	764.63	Joback Method
dvisc	0.0001297	Paxs	706.78	Joback Method
dvisc	0.0001920	Paxs	648.92	Joback Method
dvisc	0.0003069	Paxs	591.07	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344594&Units=SI

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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