

Isophthalic acid, 3-chlorophenyl hexyl ester

Inchi:	InChI=1S/C20H21ClO4/c1-2-3-4-5-12-24-19(22)15-8-6-9-16(13-15)20(23)25-18-11-7-10
InchiKey:	XXKLODQVGMZVSM-UHFFFAOYSA-N
Formula:	C20H21ClO4
SMILES:	CCCCCCOC(=O)c1cccc(C(=O)Oc2cccc(Cl)c2)c1
Mol. weight [g/mol]:	360.83

Physical Properties

Property code	Value	Unit	Source
gf	-156.69	kJ/mol	Joback Method
hf	-511.35	kJ/mol	Joback Method
hfus	44.63	kJ/mol	Joback Method
hvap	88.69	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.296		Crippen Method
mvol	272.260	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	2866.00		NIST Webbook
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tb	910.33	K	Joback Method
tc	1138.42	K	Joback Method
tf	567.28	K	Joback Method
vc	1.036	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.40	J/molxK	910.33	Joback Method
cpg	816.11	J/molxK	948.34	Joback Method
cpg	827.53	J/molxK	986.36	Joback Method
cpg	837.71	J/molxK	1024.37	Joback Method
cpg	846.69	J/molxK	1062.39	Joback Method
cpg	854.49	J/molxK	1100.40	Joback Method
cpg	861.16	J/molxK	1138.42	Joback Method
dvisc	0.0003793	Paxs	567.28	Joback Method

dvisc	0.0002313	Paxs	624.46	Joback Method
dvisc	0.0001532	Paxs	681.63	Joback Method
dvisc	0.0001082	Paxs	738.81	Joback Method
dvisc	0.0000803	Paxs	795.98	Joback Method
dvisc	0.0000620	Paxs	853.15	Joback Method
dvisc	0.0000495	Paxs	910.33	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=U344605&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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