

Isophthalic acid, 3-chlorophenyl pentyl ester

Inchi:	InChI=1S/C19H19ClO4/c1-2-3-4-11-23-18(21)14-7-5-8-15(12-14)19(22)24-17-10-6-9-16
InchiKey:	IAHULIFNMAGOQJ-UHFFFAOYSA-N
Formula:	C19H19ClO4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)Oc2cccc(Cl)c2)c1
Mol. weight [g/mol]:	346.81

Physical Properties

Property code	Value	Unit	Source
gf	-165.11	kJ/mol	Joback Method
hf	-490.71	kJ/mol	Joback Method
hfus	42.04	kJ/mol	Joback Method
hvap	86.46	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	4.906		Crippen Method
mcvol	258.170	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinsol	2762.00		NIST Webbook
tb	887.45	K	Joback Method
tc	1117.22	K	Joback Method
tf	556.01	K	Joback Method
vc	0.981	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.25	J/molxK	887.45	Joback Method
cpg	758.85	J/molxK	925.75	Joback Method
cpg	770.20	J/molxK	964.04	Joback Method
cpg	780.32	J/molxK	1002.34	Joback Method
cpg	789.24	J/molxK	1040.63	Joback Method
cpg	797.01	J/molxK	1078.93	Joback Method
cpg	803.66	J/molxK	1117.22	Joback Method
dvisc	0.0004190	Paxs	556.01	Joback Method
dvisc	0.0002585	Paxs	611.25	Joback Method

dvisc	0.0001728	Paxs	666.49	Joback Method
dvisc	0.0001228	Paxs	721.73	Joback Method
dvisc	0.0000917	Paxs	776.97	Joback Method
dvisc	0.0000711	Paxs	832.21	Joback Method
dvisc	0.0000569	Paxs	887.45	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=U344603&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
mccvol:	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

Latest version available from:

<https://www.chemeo.com/cid/99-725-8/Isophthalic-acid-3-chlorophenyl-pentyl-ester.pdf>

Generated by Cheméo on 2024-12-12 13:48:03.20494443 +0000 UTC m=+8592145.841913679.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.