

Isophthalic acid, 3-chlorophenyl propyl ester

Inchi:	InChI=1S/C17H15ClO4/c1-2-9-21-16(19)12-5-3-6-13(10-12)17(20)22-15-8-4-7-14(18)11-
InchiKey:	RGLVTEZWGQELQW-UHFFFAOYSA-N
Formula:	C17H15ClO4
SMILES:	CCCOC(=O)c1cccc(C(=O)Oc2cccc(Cl)c2)c1
Mol. weight [g/mol]:	318.75

Physical Properties

Property code	Value	Unit	Source
gf	-181.95	kJ/mol	Joback Method
hf	-449.43	kJ/mol	Joback Method
hfus	36.86	kJ/mol	Joback Method
hvap	82.01	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.126		Crippen Method
mvol	229.990	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	2551.00		NIST Webbook
rinpol	2551.00		NIST Webbook
tb	841.69	K	Joback Method
tc	1076.92	K	Joback Method
tf	533.47	K	Joback Method
vc	0.869	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.29	J/molxK	841.69	Joback Method
cpg	646.57	J/molxK	880.89	Joback Method
cpg	657.64	J/molxK	920.10	Joback Method
cpg	667.53	J/molxK	959.30	Joback Method
cpg	676.24	J/molxK	998.51	Joback Method
cpg	683.82	J/molxK	1037.71	Joback Method
cpg	690.29	J/molxK	1076.92	Joback Method
dvisc	0.0005049	Paxs	533.47	Joback Method

dvisc	0.0003193	Paxs	584.84	Joback Method
dvisc	0.0002174	Paxs	636.21	Joback Method
dvisc	0.0001568	Paxs	687.58	Joback Method
dvisc	0.0001183	Paxs	738.95	Joback Method
dvisc	0.0000926	Paxs	790.32	Joback Method
dvisc	0.0000747	Paxs	841.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344600&Units=SI
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

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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