

Isophthalic acid, di(3,5-dichlorophenyl) ester

Inchi:	InChI=1S/C20H10Cl4O4/c21-13-5-14(22)8-17(7-13)27-19(25)11-2-1-3-12(4-11)20(26)28
InchiKey:	FLGNSODEINIEOX-UHFFFAOYSA-N
Formula:	C20H10Cl4O4
SMILES:	O=C(Oc1cc(Cl)cc(Cl)c1)c1cccc(C(=O)Oc2cc(Cl)cc(Cl)c2)c1
Mol. weight [g/mol]:	456.10

Physical Properties

Property code	Value	Unit	Source
gf	-108.96	kJ/mol	Joback Method
hf	-356.45	kJ/mol	Joback Method
hfus	50.10	kJ/mol	Joback Method
hvap	106.10	kJ/mol	Joback Method
log10ws	-8.39		Crippen Method
logp	6.739		Crippen Method
mcvol	285.220	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	3525.00		NIST Webbook
rinpol	3525.00		NIST Webbook
tb	1064.24	K	Joback Method
tc	1332.44	K	Joback Method
tf	721.02	K	Joback Method
vc	1.075	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.89	J/molxK	1064.24	Joback Method
cpg	744.33	J/molxK	1108.94	Joback Method
cpg	748.36	J/molxK	1153.64	Joback Method
cpg	751.01	J/molxK	1198.34	Joback Method
cpg	752.34	J/molxK	1243.04	Joback Method
cpg	752.38	J/molxK	1287.74	Joback Method
cpg	751.20	J/molxK	1332.44	Joback Method
dvisc	0.0001611	Paxs	721.02	Joback Method

dvisc	0.0001132	Paxs	778.22	Joback Method
dvisc	0.0000835	Paxs	835.43	Joback Method
dvisc	0.0000641	Paxs	892.63	Joback Method
dvisc	0.0000507	Paxs	949.83	Joback Method
dvisc	0.0000412	Paxs	1007.04	Joback Method
dvisc	0.0000343	Paxs	1064.24	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=U356590&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

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