

Isophthalic acid, di(2-chlorophenyl) ester

Inchi: InChI=1S/C20H12Cl2O4/c21-15-8-1-3-10-17(15)25-19(23)13-6-5-7-14(12-13)20(24)26-1
InchiKey: LAGGQUMAVSOYLA-UHFFFAOYSA-N
Formula: C20H12Cl2O4
SMILES: O=C(Oc1ccccc1Cl)c1cccc(C(=O)Oc2ccccc2Cl)c1
Mol. weight [g/mol]: 387.21

Physical Properties

Property code	Value	Unit	Source
gf	-65.84	kJ/mol	Joback Method
hf	-302.03	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	96.01	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.432		Crippen Method
mvol	260.740	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	3232.00		NIST Webbook
rinpol	3232.00		NIST Webbook
tb	979.42	K	Joback Method
tc	1241.84	K	Joback Method
tf	636.14	K	Joback Method
vc	0.978	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.74	J/molxK	979.42	Joback Method
cpg	743.69	J/molxK	1198.11	Joback Method
cpg	740.32	J/molxK	1154.37	Joback Method
cpg	735.69	J/molxK	1110.63	Joback Method
cpg	729.76	J/molxK	1066.89	Joback Method
cpg	722.47	J/molxK	1023.16	Joback Method
cpg	745.87	J/molxK	1241.84	Joback Method
dvisc	0.0000450	Paxs	979.42	Joback Method

dvisc	0.0000552	Paxs	922.21	Joback Method
dvisc	0.0000696	Paxs	864.99	Joback Method
dvisc	0.0000905	Paxs	807.78	Joback Method
dvisc	0.0001227	Paxs	750.57	Joback Method
dvisc	0.0001748	Paxs	693.35	Joback Method
dvisc	0.0002654	Paxs	636.14	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=U344501&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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