Isophthalic acid, monochloride, 2-biphenyl ester

Inchi: InChI=1S/C20H13ClO3/c21-19(22)15-9-6-10-16(13-15)20(23)24-18-12-5-4-11-17(18)14-

InchiKey: QDHKTUJFUZDDEA-UHFFFAOYSA-N

Formula: C20H13ClO3

SMILES: O=C(Cl)c1cccc(C(=O)Oc2ccccc2-c2ccccc2)c1

Mol. weight [g/mol]: 336.77

Physical Properties

Property code	Value	Unit	Source
gf	60.72	kJ/mol	Joback Method
hf	-142.60	kJ/mol	Joback Method
hfus	37.48	kJ/mol	Joback Method
hvap	88.55	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	4.952		Crippen Method
mcvol	242.630	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	2714.00		NIST Webbook
rinpol	2714.00		NIST Webbook
tb	914.59	K	Joback Method
tc	1178.04	K	Joback Method
tf	571.47	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.59	J/mol×K	914.59	Joback Method
cpg	717.46	J/mol×K	1134.13	Joback Method
cpg	711.01	J/mol×K	1090.22	Joback Method
cpg	703.49	J/mol×K	1046.32	Joback Method
cpg	694.81	J/mol×K	1002.41	Joback Method
cpg	684.88	J/mol×K	958.50	Joback Method
cpg	722.95	J/mol×K	1178.04	Joback Method
dvisc	0.0000682	Pa×s	914.59	Joback Method

dvisc	0.0000847	Pa×s	857.40	Joback Method
dvisc	0.0001086	Pa×s	800.22	Joback Method
dvisc	0.0001446	Pa×s	743.03	Joback Method
dvisc	0.0002019	Pa×s	685.84	Joback Method
dvisc	0.0002997	Pa×s	628.66	Joback Method
dvisc	0.0004813	Pa×s	571.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U344574&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