Isophthalic acid, 2,6-dichlorophenyl ethyl ester

Inchi: InChI=1S/C16H12Cl2O4/c1-2-21-15(19)10-5-3-6-11(9-10)16(20)22-14-12(17)7-4-8-13(14

InchiKey: ZAFPHHSXVIVZJU-UHFFFAOYSA-N

Formula: C16H12Cl2O4

SMILES: CCOC(=O)c1cccc(C(=O)Oc2c(Cl)cccc2Cl)c1

Mol. weight [g/mol]: 339.17

Physical Properties

Property code	Value	Unit	Source
gf	-211.93	kJ/mol	Joback Method
hf	-456.00	kJ/mol	Joback Method
hfus	38.08	kJ/mol	Joback Method
hvap	84.83	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.389		Crippen Method
mcvol	228.140	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	2534.00		NIST Webbook
rinpol	2534.00		NIST Webbook
tb	861.22	K	Joback Method
tc	1103.13	K	Joback Method
tf	564.64	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.64	J/mol×K	861.22	Joback Method
cpg	609.25	J/mol×K	901.54	Joback Method
cpg	618.67	J/mol×K	941.86	Joback Method
cpg	626.91	J/mol×K	982.17	Joback Method
cpg	634.01	J/mol×K	1022.49	Joback Method
cpg	639.97	J/mol×K	1062.81	Joback Method
cpg	644.82	J/mol×K	1103.13	Joback Method
dvisc	0.0004213	Pa×s	564.64	Joback Method

dvisc	0.0002823	Pa×s	614.07	Joback Method
dvisc	0.0002007	Pa×s	663.50	Joback Method
dvisc	0.0001497	Pa×s	712.93	Joback Method
dvisc	0.0001159	Pa×s	762.36	Joback Method
dvisc	0.0000926	Pa×s	811.79	Joback Method
dvisc	0.0000759	Pa×s	861.22	Joback Method

Sources

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=U344618&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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