Isophthalic acid, 3,5-dichlorophenyl propyl ester

Inchi: InChI=1S/C17H14Cl2O4/c1-2-6-22-16(20)11-4-3-5-12(7-11)17(21)23-15-9-13(18)8-14(19

InchiKey: MUHJEZFBRASMMS-UHFFFAOYSA-N

Formula: C17H14Cl2O4

SMILES: CCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)cc(Cl)c2)c1

Mol. weight [g/mol]: 353.20

Physical Properties

Property code	Value	Unit	Source
gf	-203.51	kJ/mol	Joback Method
hf	-476.64	kJ/mol	Joback Method
hfus	40.67	kJ/mol	Joback Method
hvap	87.06	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.779		Crippen Method
mcvol	242.230	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	2633.00		NIST Webbook
rinpol	2633.00		NIST Webbook
tb	884.10	K	Joback Method
tc	1122.62	K	Joback Method
tf	575.91	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.59	J/mol×K	884.10	Joback Method
cpg	695.80	J/mol×K	1082.87	Joback Method
cpg	689.70	J/mol×K	1043.11	Joback Method
cpg	682.45	J/mol×K	1003.36	Joback Method
cpg	674.03	J/mol×K	963.61	Joback Method
cpg	664.42	J/mol×K	923.85	Joback Method
cpg	700.78	J/mol×K	1122.62	Joback Method
dvisc	0.0000663	Pa×s	884.10	Joback Method

dvisc	0.0000811	Pa×s	832.73	Joback Method
dvisc	0.0001020	Pa×s	781.37	Joback Method
dvisc	0.0001325	Pa×s	730.00	Joback Method
dvisc	0.0001791	Pa×s	678.64	Joback Method
dvisc	0.0002542	Pa×s	627.28	Joback Method
dvisc	0.0003841	Pa×s	575.91	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=U356580&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