Isophthalic acid, 4-chloro-2-methylphenyl ethyl ester

Inchi: InChI=1S/C17H15ClO4/c1-3-21-16(19)12-5-4-6-13(10-12)17(20)22-15-8-7-14(18)9-11(15

InchiKey: HQNVRKYWKQHTIP-UHFFFAOYSA-N

Formula: C17H15ClO4

SMILES: CCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2C)c1

Mol. weight [g/mol]: 318.75

Physical Properties

Property code	Value	Unit	Source
gf	-191.58	kJ/mol	Joback Method
hf	-460.90	kJ/mol	Joback Method
hfus	36.47	kJ/mol	Joback Method
hvap	82.67	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.044		Crippen Method
mcvol	229.990	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook
tb	846.67	K	Joback Method
tc	1082.61	K	Joback Method
tf	545.99	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.80	J/mol×K	846.67	Joback Method
cpg	644.99	J/mol×K	885.99	Joback Method
cpg	655.96	J/mol×K	925.32	Joback Method
cpg	665.73	J/mol×K	964.64	Joback Method
cpg	674.32	J/mol×K	1003.97	Joback Method
cpg	681.75	J/mol×K	1043.29	Joback Method
cpg	688.03	J/mol×K	1082.61	Joback Method
dvisc	0.0004480	Pa×s	545.99	Joback Method

dvisc	0.0002942	Pa×s	596.10	Joback Method
dvisc	0.0002062	Pa×s	646.22	Joback Method
dvisc	0.0001521	Pa×s	696.33	Joback Method
dvisc	0.0001169	Pa×s	746.44	Joback Method
dvisc	0.0000928	Pa×s	796.56	Joback Method
dvisc	0.0000758	Pa×s	846.67	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=U344643&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