

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

Inchi:	InChI=1S/C18H17ClO4/c1-3-9-22-17(20)13-5-4-6-14(11-13)18(21)23-16-8-7-15(19)10-12
InchiKey:	FLFYXVXAHGDGQR-UHFFFAOYSA-N
Formula:	C18H17ClO4
SMILES:	CCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2C)c1
Mol. weight [g/mol]:	332.78

Physical Properties

Property code	Value	Unit	Source
gf	-183.16	kJ/mol	Joback Method
hf	-481.54	kJ/mol	Joback Method
hfus	39.06	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.434		Crippen Method
mcvol	244.080	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	2621.00		NIST Webbook
tb	869.55	K	Joback Method
tc	1102.44	K	Joback Method
tf	557.26	K	Joback Method
vc	0.924	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.43	J/molxK	869.55	Joback Method
cpg	738.05	J/molxK	1063.63	Joback Method
cpg	730.53	J/molxK	1024.81	Joback Method
cpg	721.82	J/molxK	986.00	Joback Method
cpg	711.92	J/molxK	947.18	Joback Method
cpg	700.80	J/molxK	908.37	Joback Method
cpg	744.41	J/molxK	1102.44	Joback Method
dvisc	0.0000664	Paxs	869.55	Joback Method
dvisc	0.0000816	Paxs	817.50	Joback Method

dvisc	0.0001033	Paxs	765.45	Joback Method
dvisc	0.0001352	Paxs	713.40	Joback Method
dvisc	0.0001846	Paxs	661.36	Joback Method
dvisc	0.0002660	Paxs	609.31	Joback Method
dvisc	0.0004102	Paxs	557.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344644&Units=SI
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

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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