

Isophthalic acid, 4-methoxyphenyl propyl ester

Inchi:	InChI=1S/C18H18O5/c1-3-11-22-17(19)13-5-4-6-14(12-13)18(20)23-16-9-7-15(21-2)8-10
InchiKey:	NHSYFFIKWVDCB-UHFFFAOYSA-N
Formula:	C18H18O5
SMILES:	CCCOC(=O)c1cccc(C(=O)Oc2ccc(OC)cc2)c1
Mol. weight [g/mol]:	314.33

Physical Properties

Property code	Value	Unit	Source
gf	-266.60	kJ/mol	Joback Method
hf	-586.55	kJ/mol	Joback Method
hfus	36.44	kJ/mol	Joback Method
hvap	82.26	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.481		Crippen Method
mvol	237.710	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	2667.00		NIST Webbook
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tb	849.56	K	Joback Method
tc	1077.01	K	Joback Method
tf	537.05	K	Joback Method
vc	0.893	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.56	J/molxK	849.56	Joback Method
cpg	706.79	J/molxK	887.47	Joback Method
cpg	718.71	J/molxK	925.38	Joback Method
cpg	729.32	J/molxK	963.28	Joback Method
cpg	738.65	J/molxK	1001.19	Joback Method
cpg	746.68	J/molxK	1039.10	Joback Method
cpg	753.43	J/molxK	1077.01	Joback Method
dvisc	0.0003908	Paxs	537.05	Joback Method

dvisc	0.0002454	Paxs	589.13	Joback Method
dvisc	0.0001661	Paxs	641.22	Joback Method
dvisc	0.0001193	Paxs	693.31	Joback Method
dvisc	0.0000897	Paxs	745.39	Joback Method
dvisc	0.0000700	Paxs	797.47	Joback Method
dvisc	0.0000563	Paxs	849.56	Joback Method

Sources

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=U344476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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