

Isophthalic acid, 4-methoxybenzyl propyl ester

Inchi:	InChI=1S/C19H20O5/c1-3-11-23-18(20)15-5-4-6-16(12-15)19(21)24-13-14-7-9-17(22-2)
InchiKey:	PRZDDXRMVIFYQB-UHFFFAOYSA-N
Formula:	C19H20O5
SMILES:	CCCOC(=O)c1cccc(C(=O)OCc2ccc(OC)cc2)c1
Mol. weight [g/mol]:	328.36

Physical Properties

Property code	Value	Unit	Source
gf	-258.18	kJ/mol	Joback Method
hf	-607.19	kJ/mol	Joback Method
hfus	39.03	kJ/mol	Joback Method
hvap	84.49	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	3.619		Crippen Method
mcvol	251.800	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
rinpol	2743.00		NIST Webbook
tb	872.44	K	Joback Method
tc	1097.71	K	Joback Method
tf	548.32	K	Joback Method
vc	0.950	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.17	J/molxK	872.44	Joback Method
cpg	803.43	J/molxK	1060.16	Joback Method
cpg	795.42	J/molxK	1022.62	Joback Method
cpg	786.10	J/molxK	985.07	Joback Method
cpg	775.46	J/molxK	947.53	Joback Method
cpg	763.48	J/molxK	909.98	Joback Method
cpg	810.15	J/molxK	1097.71	Joback Method
dvisc	0.0000492	Paxs	872.44	Joback Method
dvisc	0.0000614	Paxs	818.42	Joback Method

dvisc	0.0000790	Paxs	764.40	Joback Method
dvisc	0.0001057	Paxs	710.38	Joback Method
dvisc	0.0001483	Paxs	656.36	Joback Method
dvisc	0.0002211	Paxs	602.34	Joback Method
dvisc	0.0003565	Paxs	548.32	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=U344383&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

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