

Isophthalic acid, 2,6-dimethoxyphenyl propyl ester

Inchi:	InChI=1S/C19H20O6/c1-4-11-24-18(20)13-7-5-8-14(12-13)19(21)25-17-15(22-2)9-6-10-
InchiKey:	AQHCTGJEARXVSV-UHFFFAOYSA-N
Formula:	C19H20O6
SMILES:	CCCOC(=O)c1cccc(C(=O)Oc2c(OC)cccc2OC)c1
Mol. weight [g/mol]:	344.36

Physical Properties

Property code	Value	Unit	Source
gf	-372.81	kJ/mol	Joback Method
hf	-750.88	kJ/mol	Joback Method
hfus	39.83	kJ/mol	Joback Method
hvap	87.56	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.490		Crippen Method
mcvol	257.670	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinsol	2745.00		NIST Webbook
tb	899.84	K	Joback Method
tc	1125.04	K	Joback Method
tf	583.07	K	Joback Method
vc	0.968	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.52	J/molxK	899.84	Joback Method
cpg	787.95	J/molxK	937.37	Joback Method
cpg	798.91	J/molxK	974.91	Joback Method
cpg	808.40	J/molxK	1012.44	Joback Method
cpg	816.40	J/molxK	1049.97	Joback Method
cpg	822.89	J/molxK	1087.51	Joback Method
cpg	827.86	J/molxK	1125.04	Joback Method
dvisc	0.0002295	Paxs	583.07	Joback Method
dvisc	0.0001498	Paxs	635.87	Joback Method

dvisc	0.0001045	Paxs	688.66	Joback Method
dvisc	0.0000766	Paxs	741.45	Joback Method
dvisc	0.0000586	Paxs	794.25	Joback Method
dvisc	0.0000463	Paxs	847.04	Joback Method
dvisc	0.0000377	Paxs	899.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344531&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

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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