

Isophthalic acid, ethyl 2-isopropoxyphenyl ester

Inchi:	InChI=1S/C19H20O5/c1-4-22-18(20)14-8-7-9-15(12-14)19(21)24-17-11-6-5-10-16(17)23
InchiKey:	YIYFMMIVPWKTLV-UHFFFAOYSA-N
Formula:	C19H20O5
SMILES:	CCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)c1
Mol. weight [g/mol]:	328.36

Physical Properties

Property code	Value	Unit	Source
gf	-260.62	kJ/mol	Joback Method
hf	-612.47	kJ/mol	Joback Method
hfus	35.51	kJ/mol	Joback Method
hvap	84.10	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	3.870		Crippen Method
mcvol	251.800	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinsol	2478.00		NIST Webbook
tb	872.00	K	Joback Method
tc	1100.23	K	Joback Method
tf	533.32	K	Joback Method
vc	0.944	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.72	J/molxK	872.00	Joback Method
cpg	764.18	J/molxK	910.04	Joback Method
cpg	776.25	J/molxK	948.08	Joback Method
cpg	786.94	J/molxK	986.11	Joback Method
cpg	796.26	J/molxK	1024.15	Joback Method
cpg	804.23	J/molxK	1062.19	Joback Method
cpg	810.84	J/molxK	1100.23	Joback Method
dvisc	0.0003889	Paxs	533.32	Joback Method
dvisc	0.0002286	Paxs	589.77	Joback Method

dvisc	0.0001475	Paxs	646.21	Joback Method
dvisc	0.0001021	Paxs	702.66	Joback Method
dvisc	0.0000746	Paxs	759.11	Joback Method
dvisc	0.0000570	Paxs	815.55	Joback Method
dvisc	0.0000450	Paxs	872.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344425&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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