

Isophthalic acid, ethyl 2-methylphenyl ester

Inchi:	InChI=1S/C17H16O4/c1-3-20-16(18)13-8-6-9-14(11-13)17(19)21-15-10-5-4-7-12(15)2/h4
InchiKey:	TUNXCWLFCLBHKT-UHFFFAOYSA-N
Formula:	C17H16O4
SMILES:	CCOC(=O)c1cccc(C(=O)Oc2ccccc2C)c1
Mol. weight [g/mol]:	284.31

Physical Properties

Property code	Value	Unit	Source
gf	-170.02	kJ/mol	Joback Method
hf	-433.69	kJ/mol	Joback Method
hfus	32.66	kJ/mol	Joback Method
hvap	77.62	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.391		Crippen Method
mvol	217.750	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	2309.00		NIST Webbook
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tb	804.26	K	Joback Method
tc	1036.96	K	Joback Method
tf	503.55	K	Joback Method
vc	0.820	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.57	J/molxK	804.26	Joback Method
cpg	625.23	J/molxK	843.04	Joback Method
cpg	637.67	J/molxK	881.83	Joback Method
cpg	648.92	J/molxK	920.61	Joback Method
cpg	658.98	J/molxK	959.39	Joback Method
cpg	667.89	J/molxK	998.17	Joback Method
cpg	675.67	J/molxK	1036.96	Joback Method
dvisc	0.0005863	Paxs	503.55	Joback Method

dvisc	0.0003666	Paxs	553.67	Joback Method
dvisc	0.0002478	Paxs	603.79	Joback Method
dvisc	0.0001779	Paxs	653.90	Joback Method
dvisc	0.0001339	Paxs	704.02	Joback Method
dvisc	0.0001046	Paxs	754.14	Joback Method
dvisc	0.0000843	Paxs	804.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344344&Units=SI

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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