

Isophthalic acid, ethyl 3-phenylpropyl ester

Inchi:	InChI=1S/C19H20O4/c1-2-22-18(20)16-11-6-12-17(14-16)19(21)23-13-7-10-15-8-4-3-5-9
InchiKey:	DGWSPKHWLFOOA-UHFFFAOYSA-N
Formula:	C19H20O4
SMILES:	CCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
Mol. weight [g/mol]:	312.36

Physical Properties

Property code	Value	Unit	Source
gf	-143.55	kJ/mol	Joback Method
hf	-463.50	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	81.41	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.653		Crippen Method
mvol	245.930	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	845.04	K	Joback Method
tc	1070.91	K	Joback Method
tf	513.57	K	Joback Method
vc	0.931	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.43	J/molxK	845.04	Joback Method
cpg	738.52	J/molxK	882.69	Joback Method
cpg	751.35	J/molxK	920.33	Joback Method
cpg	762.96	J/molxK	957.98	Joback Method
cpg	773.37	J/molxK	995.62	Joback Method
cpg	782.63	J/molxK	1033.27	Joback Method
cpg	790.77	J/molxK	1070.91	Joback Method
dvisc	0.0005675	Paxs	513.57	Joback Method

dvisc	0.0003309	Paxs	568.81	Joback Method
dvisc	0.0002123	Paxs	624.06	Joback Method
dvisc	0.0001464	Paxs	679.30	Joback Method
dvisc	0.0001068	Paxs	734.55	Joback Method
dvisc	0.0000814	Paxs	789.79	Joback Method
dvisc	0.0000643	Paxs	845.04	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=U344385&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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