

Isophthalic acid, ethyl 1-phenylpropyl ester

Inchi:	InChI=1S/C19H20O4/c1-3-17(14-9-6-5-7-10-14)23-19(21)16-12-8-11-15(13-16)18(20)22
InchiKey:	QCQQWHIMVURXKR-UHFFFAOYSA-N
Formula:	C19H20O4
SMILES:	CCOC(=O)c1cccc(C(=O)OC(CC)c2ccccc2)c1
Mol. weight [g/mol]:	312.36

Physical Properties

Property code	Value	Unit	Source
gf	-145.99	kJ/mol	Joback Method
hf	-468.78	kJ/mol	Joback Method
hfus	34.71	kJ/mol	Joback Method
hvap	81.03	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.171		Crippen Method
mvol	245.930	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	2431.00		NIST Webbook
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tb	844.60	K	Joback Method
tc	1073.74	K	Joback Method
tf	498.57	K	Joback Method
vc	0.925	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.99	J/molxK	844.60	Joback Method
cpg	739.26	J/molxK	882.79	Joback Method
cpg	752.23	J/molxK	920.98	Joback Method
cpg	763.91	J/molxK	959.17	Joback Method
cpg	774.36	J/molxK	997.36	Joback Method
cpg	783.61	J/molxK	1035.55	Joback Method
cpg	791.70	J/molxK	1073.74	Joback Method
dvisc	0.0006328	Paxs	498.57	Joback Method

dvisc	0.0003470	Paxs	556.24	Joback Method
dvisc	0.0002130	Paxs	613.91	Joback Method
dvisc	0.0001422	Paxs	671.59	Joback Method
dvisc	0.0001012	Paxs	729.26	Joback Method
dvisc	0.0000757	Paxs	786.93	Joback Method
dvisc	0.0000589	Paxs	844.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344547&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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