

Isophthalic acid, 3,4-dimethylphenyl propyl ester

Inchi:	InChI=1S/C19H20O4/c1-4-10-22-18(20)15-6-5-7-16(12-15)19(21)23-17-9-8-13(2)14(3)1
InchiKey:	WUCWVYNEMBICDK-UHFFFAOYSA-N
Formula:	C19H20O4
SMILES:	CCCOC(=O)c1cccc(C(=O)Oc2ccc(C)c(C)c2)c1
Mol. weight [g/mol]:	312.36

Physical Properties

Property code	Value	Unit	Source
gf	-162.81	kJ/mol	Joback Method
hf	-486.44	kJ/mol	Joback Method
hfus	37.45	kJ/mol	Joback Method
hvap	82.74	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.089		Crippen Method
mcvol	245.930	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinsol	2575.00		NIST Webbook
tb	855.00	K	Joback Method
tc	1082.36	K	Joback Method
tf	538.61	K	Joback Method
vc	0.931	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.06	J/mol×K	855.00	Joback Method
cpg	735.95	J/mol×K	892.89	Joback Method
cpg	748.57	J/mol×K	930.79	Joback Method
cpg	759.95	J/mol×K	968.68	Joback Method
cpg	770.09	J/mol×K	1006.57	Joback Method
cpg	779.04	J/mol×K	1044.46	Joback Method
cpg	786.80	J/mol×K	1082.36	Joback Method
dvisc	0.0004374	Paxs	538.61	Joback Method
dvisc	0.0002774	Paxs	591.34	Joback Method

dvisc	0.0001896	Paxs	644.07	Joback Method
dvisc	0.0001373	Paxs	696.81	Joback Method
dvisc	0.0001040	Paxs	749.54	Joback Method
dvisc	0.0000817	Paxs	802.27	Joback Method
dvisc	0.0000662	Paxs	855.00	Joback Method

Sources

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=U344439&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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