

Isophthalic acid, ethyl 3-methylpentyl ester

Inchi:	InChI=1S/C16H22O4/c1-4-12(3)9-10-20-16(18)14-8-6-7-13(11-14)15(17)19-5-2/h6-8,11-
InchiKey:	FGSUDAUHMDTHKE-UHFFFAOYSA-N
Formula:	C16H22O4
SMILES:	CCOC(=O)c1cccc(C(=O)OCCC(C)CC)c1
Mol. weight [g/mol]:	278.34

Physical Properties

Property code	Value	Unit	Source
gf	-283.66	kJ/mol	Joback Method
hf	-643.39	kJ/mol	Joback Method
hfus	32.90	kJ/mol	Joback Method
hvap	72.07	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.456		Crippen Method
mvol	227.420	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	749.28	K	Joback Method
tc	954.00	K	Joback Method
tf	438.34	K	Joback Method
vc	0.866	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.00	J/molxK	749.28	Joback Method
cpg	664.35	J/molxK	783.40	Joback Method
cpg	678.69	J/molxK	817.52	Joback Method
cpg	692.04	J/molxK	851.64	Joback Method
cpg	704.40	J/molxK	885.76	Joback Method
cpg	715.80	J/molxK	919.88	Joback Method
cpg	726.23	J/molxK	954.00	Joback Method
dvisc	0.0009839	Paxs	438.34	Joback Method

dvisc	0.0005289	Paxs	490.16	Joback Method
dvisc	0.0003201	Paxs	541.99	Joback Method
dvisc	0.0002115	Paxs	593.81	Joback Method
dvisc	0.0001494	Paxs	645.63	Joback Method
dvisc	0.0001111	Paxs	697.46	Joback Method
dvisc	0.0000861	Paxs	749.28	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=U356539&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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