

Isophthalic acid, di(3-methylbut-2-yl) ester

Inchi:	InChI=1S/C18H26O4/c1-11(2)13(5)21-17(19)15-8-7-9-16(10-15)18(20)22-14(6)12(3)4/h
InchiKey:	ZYTDGEGICDUKCZ-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CC(C)C(C)OC(=O)c1cccc(C(=O)OC(C)C(C)C)c1
Mol. weight [g/mol]:	306.40

Physical Properties

Property code	Value	Unit	Source
gf	-274.14	kJ/mol	Joback Method
hf	-700.51	kJ/mol	Joback Method
hfus	27.51	kJ/mol	Joback Method
hvap	75.36	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.089		Crippen Method
mvol	255.600	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	2124.00		NIST Webbook
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tb	793.72	K	Joback Method
tc	1003.71	K	Joback Method
tf	415.88	K	Joback Method
vc	0.960	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.39	J/molxK	793.72	Joback Method
cpg	779.87	J/molxK	828.72	Joback Method
cpg	795.15	J/molxK	863.72	Joback Method
cpg	809.25	J/molxK	898.71	Joback Method
cpg	822.19	J/molxK	933.71	Joback Method
cpg	833.99	J/molxK	968.71	Joback Method
cpg	844.67	J/molxK	1003.71	Joback Method
dvisc	0.0013805	Paxs	415.88	Joback Method

dvisc	0.0005561	Paxs	478.85	Joback Method
dvisc	0.0002768	Paxs	541.83	Joback Method
dvisc	0.0001593	Paxs	604.80	Joback Method
dvisc	0.0001017	Paxs	667.77	Joback Method
dvisc	0.0000702	Paxs	730.75	Joback Method
dvisc	0.0000514	Paxs	793.72	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=U344726&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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