

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C18H26O4/c1-11(2)13(5)21-17(19)15-7-9-16(10-8-15)18(20)22-14(6)12(3)4/h7-10,12-14,16-20,22H

IJLDTTKUGDCXNJ-UHFFFAOYSA-N

C18H26O4

CC(C)C(C)OC(=O)c1ccc(C(=O)OC(C)C(C)C)cc1

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
mcvol	255.600	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	2069.00		NIST Webbook
rinpol	2069.00		NIST Webbook
tb	793.72	K	Joback Method
tc	1003.71	K	Joback Method
tf	415.88	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.39	J/mol×K	793.72	Joback Method
cpg	833.99	J/mol×K	968.71	Joback Method
cpg	822.19	J/mol×K	933.71	Joback Method
cpg	809.25	J/mol×K	898.71	Joback Method
cpg	795.15	J/mol×K	863.72	Joback Method
cpg	779.87	J/mol×K	828.72	Joback Method
cpg	844.67	J/mol×K	1003.71	Joback Method
dvisc	0.0000514	Pa×s	793.72	Joback Method

dvisc	0.0000702	Pa×s	730.75	Joback Method
dvisc	0.0001017	Pa×s	667.77	Joback Method
dvisc	0.0001593	Pa×s	604.80	Joback Method
dvisc	0.0002768	Pa×s	541.83	Joback Method
dvisc	0.0005561	Pa×s	478.85	Joback Method
dvisc	0.0013805	Pa×s	415.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U356270&Units=SI

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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