Terephthalic acid, isobutyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C17H24O4/c1-11(2)10-20-16(18)14-6-8-15(9-7-14)17(19)21-13(5)12(3)4/h6-9,
InchiKey: BRFJQOMPAMZMGW-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: CC(C)COC(=O)c1ccc(C(=O)OC(C)C(C)C)cc1
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-280.12	kJ/mol	Joback Method
hf	-674.59	kJ/mol	Joback Method
hfus	28.44	kJ/mol	Joback Method
hvap	73.52	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.701		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	2023.00		NIST Webbook
rinpol	2023.00		NIST Webbook
tb	771.28	K	Joback Method
tc	980.14	K	Joback Method
tf	419.61	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.98	J/mol×K	771.28	Joback Method
cpg	722.05	J/mol×K	806.09	Joback Method
cpg	737.00	J/mol×K	840.90	Joback Method
cpg	750.84	J/mol×K	875.71	Joback Method
cpg	763.59	J/mol×K	910.52	Joback Method
cpg	775.27	J/mol×K	945.33	Joback Method
cpg	785.88	J/mol×K	980.14	Joback Method
dvisc	0.0012619	Pa×s	419.61	Joback Method

dvisc	0.0005663	Pa×s	478.22	Joback Method
dvisc	0.0003027	Pa×s	536.83	Joback Method
dvisc	0.0001830	Pa×s	595.45	Joback Method
dvisc	0.0001211	Pa×s	654.06	Joback Method
dvisc	0.0000858	Pa×s	712.67	Joback Method
dvisc	0.0000640	Pa×s	771.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356271&Units=SI
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

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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