Terephthalic acid, di(4-methylpent-2-yl) ester

Inchi: InChI=1S/C20H30O4/c1-13(2)11-15(5)23-19(21)17-7-9-18(10-8-17)20(22)24-16(6)12-14
InchiKey: KSTYDRQJWZTRRO-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CC(C)CC(C)OC(=O)c1ccc(C(=O)OC(C)CC(C)C)cc1
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-257.30	kJ/mol	Joback Method
hf	-741.79	kJ/mol	Joback Method
hfus	32.69	kJ/mol	Joback Method
hvap	79.81	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.869		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
tb	839.48	K	Joback Method
tc	1047.32	K	Joback Method
tf	438.42	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.79	J/mol×K	839.48	Joback Method
cpg	896.49	J/mol×K	874.12	Joback Method
cpg	911.94	J/mol×K	908.76	Joback Method
cpg	926.15	J/mol×K	943.40	Joback Method
cpg	939.15	J/mol×K	978.04	Joback Method
cpg	950.96	J/mol×K	1012.68	Joback Method
cpg	961.60	J/mol×K	1047.32	Joback Method
dvisc	0.0010900	Pa×s	438.42	Joback Method

dvisc	0.0004325	Pa×s	505.26	Joback Method
dvisc	0.0002129	Pa×s	572.11	Joback Method
dvisc	0.0001216	Pa×s	638.95	Joback Method
dvisc	0.0000772	Pa×s	705.79	Joback Method
dvisc	0.0000530	Pa×s	772.64	Joback Method
dvisc	0.0000387	Pa×s	839.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356264&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