Phthalic acid, di(2,2-dimethylpent-3-yl) ester

Inchi: InChI=1S/C22H34O4/c1-9-17(21(3,4)5)25-19(23)15-13-11-12-14-16(15)20(24)26-18(10-
InchiKey: OUAIKFCXUVPKPJ-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CCC(OC(=O)c1ccccc1C(=O)OC(CC)C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-229.90	kJ/mol	Joback Method
hf	-790.01	kJ/mol	Joback Method
hfus	30.09	kJ/mol	Joback Method
hvap	82.45	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.650		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1215.74	kPa	Joback Method
rinpol	1577.00		NIST Webbook
rinpol	1577.00		NIST Webbook
tb	879.66	K	Joback Method
tc	1094.58	K	Joback Method
tf	495.80	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.41	J/mol×K	879.66	Joback Method
cpg	1016.47	J/mol×K	915.48	Joback Method
cpg	1032.26	J/mol×K	951.30	Joback Method
cpg	1046.85	J/mol×K	987.12	Joback Method
cpg	1060.31	J/mol×K	1022.94	Joback Method
cpg	1072.71	J/mol×K	1058.76	Joback Method
cpg	1084.14	J/mol×K	1094.58	Joback Method
dvisc	0.0005260	Pa×s	495.80	Joback Method

dvisc	0.0002264	Pa×s	559.78	Joback Method
dvisc	0.0001158	Pa×s	623.75	Joback Method
dvisc	0.0000671	Pa×s	687.73	Joback Method
dvisc	0.0000427	Pa×s	751.71	Joback Method
dvisc	0.0000291	Pa×s	815.68	Joback Method
dvisc	0.0000210	Pa×s	879.66	Joback Method

Sources

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=U415538&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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