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

Inchi: InChI=1S/C22H34O4/c1-15(13-21(3,4)5)25-19(23)17-9-11-18(12-10-17)20(24)26-16(2)14

InchiKey: GVLJBXDOKCMJEJ-UHFFFAOYSA-N

Formula: C22H34O4

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

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
hfus	30.09	kJ/mol	Joback Method
ie	9.29	eV	Cheméo Relay (1.0)
log10ws	-6.10		Cheméo Relay (1.0)
logp	5.650		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
rinpol	2632.00		NIST Webbook
rinpol	2632.00		NIST Webbook
tb	625.66	K	Cheméo Relay (1.0)
tf	379.69	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.41	J/mol×K	879.66	Joback Method
cpg	1084.14	J/mol×K	1094.58	Joback Method
cpg	1072.71	J/mol×K	1058.76	Joback Method
cpg	1060.31	J/mol×K	1022.94	Joback Method
cpg	1046.85	J/mol×K	987.12	Joback Method
cpg	1032.26	J/mol×K	951.30	Joback Method
cpg	1016.47	J/mol×K	915.48	Joback Method
dvisc	0.0000671	Pa×s	687.73	Joback Method
dvisc	0.0000210	Pa×s	879.66	Joback Method
dvisc	0.0000291	Pa×s	815.68	Joback Method
dvisc	0.0000427	Pa×s	751.71	Joback Method
dvisc	0.0005260	Pa×s	495.80	Joback Method
dvisc	0.0001158	Pa×s	623.75	Joback Method

dvisc	0.0002264	Pa×s	559.78	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415958&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point