Terephthalic acid, 4,4-dimethylpent-2-yl pentyl ester

Inchi: InChI=1S/C20H30O4/c1-6-7-8-13-23-18(21)16-9-11-17(12-10-16)19(22)24-15(2)14-20(3

InchiKey: XJVMFKRXDBQFGN-UHFFFAOYSA-N

Formula: C20H30O4

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

Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
af	0.8943		Cheméo Relay (1.0)
hf	-873.20	kJ/mol	Cheméo Relay (1.0)
hfus	35.84	kJ/mol	Joback Method
hvap	92.32	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.71		Cheméo Relay (1.0)
logp	5.015		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook
tb	626.61	K	Cheméo Relay (1.0)
tc	817.01	K	Cheméo Relay (1.0)
tf	321.65	K	Cheméo Relay (1.0)
vc	1.047	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.27	J/mol×K	837.57	Joback Method
cpg	895.72	J/mol×K	872.13	Joback Method
cpg	910.98	J/mol×K	906.68	Joback Method
cpg	925.11	J/mol×K	941.24	Joback Method
cpg	938.13	J/mol×K	975.79	Joback Method
cpg	950.10	J/mol×K	1010.35	Joback Method
cpg	961.05	J/mol×K	1044.90	Joback Method
dvisc	0.0006273	Pa×s	485.84	Joback Method

dvisc	0.0003093	Pa×s	544.46	Joback Method
dvisc	0.0001750	Pa×s	603.08	Joback Method
dvisc	0.0001095	Pa×s	661.70	Joback Method
dvisc	0.0000740	Pa×s	720.33	Joback Method
dvisc	0.0000530	Pa×s	778.95	Joback Method
dvisc	0.0000398	Pa×s	837.57	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415953&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

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.