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

Inchi: InChI=1S/C23H36O4/c1-6-7-8-9-10-11-16-26-21(24)19-12-14-20(15-13-19)22(25)27-18(

InchiKey: OMZGJAPHDINKTQ-UHFFFAOYSA-N

Formula: C23H36O4

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

Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
af	1.0131		Cheméo Relay (1.0)
hf	-932.68	kJ/mol	Cheméo Relay (1.0)
hfus	43.62	kJ/mol	Joback Method
hvap	102.71	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.61		Cheméo Relay (1.0)
logp	6.185		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	2705.00		NIST Webbook
rinpol	2705.00		NIST Webbook
tb	649.70	K	Cheméo Relay (1.0)
tc	843.34	K	Cheméo Relay (1.0)
tf	324.50	K	Cheméo Relay (1.0)
vc	1.212	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.87	J/mol×K	906.21	Joback Method
cpg	1075.76	J/mol×K	941.10	Joback Method
cpg	1091.37	J/mol×K	975.98	Joback Method
cpg	1105.75	J/mol×K	1010.87	Joback Method
cpg	1118.97	J/mol×K	1045.76	Joback Method
cpg	1131.08	J/mol×K	1080.64	Joback Method
cpg	1142.12	J/mol×K	1115.53	Joback Method
dvisc	0.0004367	Pa×s	519.65	Joback Method

dvisc	0.0002089	Pa×s	584.08	Joback Method
dvisc	0.0001157	Pa×s	648.50	Joback Method
dvisc	0.0000713	Pa×s	712.93	Joback Method
dvisc	0.0000476	Pa×s	777.36	Joback Method
dvisc	0.0000338	Pa×s	841.78	Joback Method
dvisc	0.0000252	Pa×s	906.21	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415956&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

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.