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

Inchi: InChI=1S/C21H32O4/c1-6-8-9-10-15-24-19(22)16-11-13-17(14-12-16)20(23)25-18(7-2)2
InchiKey: CBOUFNZHMQHDHG-UHFFFAOYSA-N
Formula: C21H32O4
SMILES: CCCCCCOC(=O)c1ccc(C(=O)OC(CC)C(C)(C)C)cc1
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
af	0.9333		Cheméo Relay (1.0)
hf	-877.79	kJ/mol	Cheméo Relay (1.0)
hfus	38.43	kJ/mol	Joback Method
hvap	96.26	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.07		Cheméo Relay (1.0)
logp	5.405		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinpol	2507.00		NIST Webbook
rinpol	2507.00		NIST Webbook
tb	638.40	K	Cheméo Relay (1.0)
tc	834.74	K	Cheméo Relay (1.0)
tf	322.15	K	Cheméo Relay (1.0)
vc	1.091	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.43	J/mol×K	860.45	Joback Method
cpg	955.02	J/mol×K	894.99	Joback Method
cpg	970.40	J/mol×K	929.54	Joback Method
cpg	984.62	J/mol×K	964.08	Joback Method
cpg	997.72	J/mol×K	998.62	Joback Method
cpg	1009.74	J/mol×K	1033.16	Joback Method
cpg	1020.73	J/mol×K	1067.71	Joback Method
dvisc	0.0005578	Pa×s	497.11	Joback Method

dvisc	0.0002722	Pa×s	557.67	Joback Method
dvisc	0.0001529	Pa×s	618.22	Joback Method
dvisc	0.0000952	Pa×s	678.78	Joback Method
dvisc	0.0000640	Pa×s	739.34	Joback Method
dvisc	0.0000457	Pa×s	799.89	Joback Method
dvisc	0.0000343	Pa×s	860.45	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415969&Units=SI

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

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