

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

Inchi: InChI=1S/C20H30O4/c1-6-8-9-14-23-18(21)15-10-12-16(13-11-15)19(22)24-17(7-2)20(3)
InchiKey: URJMGPFJUQWNQO-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CCCCCOC(=O)c1ccc(C(=O)OC(CC)C(C)(C)C)cc1
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
af	0.8934		Cheméo Relay (1.0)
hf	-857.83	kJ/mol	Cheméo Relay (1.0)
hfus	35.84	kJ/mol	Joback Method
hvap	92.65	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.76		Cheméo Relay (1.0)
logp	5.015		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	2405.00		NIST Webbook
rinpol	2405.00		NIST Webbook
tb	630.39	K	Cheméo Relay (1.0)
tc	825.83	K	Cheméo Relay (1.0)
tf	321.48	K	Cheméo Relay (1.0)
vc	1.036	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	961.05	J/mol×K	1044.90	Joback Method
cpg	950.10	J/mol×K	1010.35	Joback Method
cpg	938.13	J/mol×K	975.79	Joback Method
cpg	925.11	J/mol×K	941.24	Joback Method
cpg	910.98	J/mol×K	906.68	Joback Method
cpg	895.72	J/mol×K	872.13	Joback Method
dvisc	0.0001095	Pa×s	661.70	Joback Method

dvisc	0.0000398	Pa×s	837.57	Joback Method
dvisc	0.0000530	Pa×s	778.95	Joback Method
dvisc	0.0000740	Pa×s	720.33	Joback Method
dvisc	0.0006273	Pa×s	485.84	Joback Method
dvisc	0.0001750	Pa×s	603.08	Joback Method
dvisc	0.0003093	Pa×s	544.46	Joback Method

Sources

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=U415968&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

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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