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

Inchi: InChI=1S/C17H24O4/c1-6-14(17(3,4)5)21-16(19)13-10-8-12(9-11-13)15(18)20-7-2/h8-11
InchiKey: ONMOCKIZPWRAMC-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: CCOC(=O)c1ccc(C(=O)OC(CC)C(C)(C)C)cc1
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-272.40	kJ/mol	Joback Method
hf	-672.78	kJ/mol	Joback Method
hfus	28.07	kJ/mol	Joback Method
hvap	73.00	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.845		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	2090.00		NIST Webbook
rinpol	2090.00		NIST Webbook
tb	768.93	K	Joback Method
tc	980.32	K	Joback Method
tf	452.03	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.75	J/mol×K	768.93	Joback Method
cpg	775.62	J/mol×K	945.08	Joback Method
cpg	763.96	J/mol×K	909.85	Joback Method
cpg	751.28	J/mol×K	874.62	Joback Method
cpg	737.54	J/mol×K	839.39	Joback Method
cpg	722.71	J/mol×K	804.16	Joback Method
cpg	786.30	J/mol×K	980.32	Joback Method
dvisc	0.0000615	Pa×s	768.93	Joback Method

dvisc	0.0000813	Pa×s	716.11	Joback Method
dvisc	0.0001123	Pa×s	663.30	Joback Method
dvisc	0.0001641	Pa×s	610.48	Joback Method
dvisc	0.0002576	Pa×s	557.66	Joback Method
dvisc	0.0004446	Pa×s	504.85	Joback Method
dvisc	0.0008716	Pa×s	452.03	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415964&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
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