Terephthalic acid, ethyl 5-methylhex-2-yl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-277.68	kJ/mol	Joback Method
hf	-669.31	kJ/mol	Joback Method
hfus	31.97	kJ/mol	Joback Method
hvap	73.91	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.845		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1699.10	kPa	Joback Method
rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook
tb	771.72	K	Joback Method
tc	977.62	K	Joback Method
tf	434.61	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.43	J/mol×K	771.72	Joback Method
cpg	721.28	J/mol×K	806.04	Joback Method
cpg	736.04	J/mol×K	840.35	Joback Method
cpg	749.74	J/mol×K	874.67	Joback Method
cpg	762.38	J/mol×K	908.99	Joback Method
cpg	773.98	J/mol×K	943.31	Joback Method
cpg	784.57	J/mol×K	977.62	Joback Method
dvisc	0.0010554	Pa×s	434.61	Joback Method

dvisc	0.0005175	Pa×s	490.80	Joback Method
dvisc	0.0002938	Pa×s	546.98	Joback Method
dvisc	0.0001853	Pa×s	603.16	Joback Method
dvisc	0.0001265	Pa×s	659.35	Joback Method
dvisc	0.0000916	Pa×s	715.54	Joback Method
dvisc	0.0000696	Pa×s	771.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382994&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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