2-Methoxyethyl 4-tert-butyl benzoate

Inchi: InChI=1S/C14H20O3/c1-14(2,3)12-7-5-11(6-8-12)13(15)17-10-9-16-4/h5-8H,9-10H2,1-4
InchiKey: JPGBDPOJLLGSQH-UHFFFAOYSA-N
Formula: C14H20O3
SMILES: COCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 236.31

Physical Properties

Property code	Value	Unit	Source
gf	-166.30	kJ/mol	Joback Method
hf	-493.00	kJ/mol	Joback Method
hfus	22.23	kJ/mol	Joback Method
hvap	59.97	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.787		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1700.00		NIST Webbook
rinpol	1700.00		NIST Webbook
tb	646.86	K	Joback Method
tc	856.76	K	Joback Method
tf	383.29	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.93	J/mol×K	646.86	Joback Method
cpg	596.48	J/mol×K	821.78	Joback Method
cpg	583.86	J/mol×K	786.80	Joback Method
cpg	570.33	J/mol×K	751.81	Joback Method
cpg	555.85	J/mol×K	716.83	Joback Method
cpg	540.39	J/mol×K	681.84	Joback Method
cpg	608.20	J/mol×K	856.76	Joback Method
dvisc	0.0001021	Pa×s	646.86	Joback Method

dvisc	0.0001329	Pa×s	602.93	Joback Method
dvisc	0.0001803	Pa×s	559.00	Joback Method
dvisc	0.0002578	Pa×s	515.07	Joback Method
dvisc	0.0003939	Pa×s	471.15	Joback Method
dvisc	0.0006566	Pa×s	427.22	Joback Method
dvisc	0.0012306	Pa×s	383.29	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540613&Units=SI

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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