Benzoic acid, 4,4-dimethylpent-2-yl ester

Inchi: InChI=1S/C14H20O2/c1-11(10-14(2,3)4)16-13(15)12-8-6-5-7-9-12/h5-9,11H,10H2,1-4H3
InchiKey: GZYLCJLBBIWGJZ-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: CC(CC(C)(C)C)OC(=O)c1ccccc1
Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
gf	-54.11	kJ/mol	Joback Method
hf	-354.59	kJ/mol	Joback Method
hfus	17.91	kJ/mol	Joback Method
hvap	56.51	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.668		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	1507.00		NIST Webbook
tb	619.02	K	Joback Method
tc	834.56	K	Joback Method
tf	333.54	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.56	J/mol×K	619.02	Joback Method
cpg	515.08	J/mol×K	654.94	Joback Method
cpg	531.45	J/mol×K	690.87	Joback Method
cpg	546.72	J/mol×K	726.79	Joback Method
cpg	560.96	J/mol×K	762.71	Joback Method
cpg	574.20	J/mol×K	798.64	Joback Method
cpg	586.51	J/mol×K	834.56	Joback Method
dvisc	0.0030275	Pa×s	333.54	Joback Method
dvisc	0.0012758	Pa×s	381.12	Joback Method

dvisc	0.0006513	Pa×s	428.70	Joback Method
dvisc	0.0003803	Pa×s	476.28	Joback Method
dvisc	0.0002449	Pa×s	523.86	Joback Method
dvisc	0.0001697	Pa×s	571.44	Joback Method
dvisc	0.0001244	Pa×s	619.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368701&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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