Benzoic acid, 4-methylpent-2-yl ester

Inchi: InChI=1S/C13H18O2/c1-10(2)9-11(3)15-13(14)12-7-5-4-6-8-12/h4-8,10-11H,9H2,1-3H3
InchiKey: WMNCKJFVKMDUJQ-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CC(C)CC(C)OC(=O)c1ccccc1
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	-67.81	kJ/mol	Joback Method
hf	-330.48	kJ/mol	Joback Method
hfus	19.21	kJ/mol	Joback Method
hvap	55.19	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.278		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1460.00		NIST Webbook
tb	598.93	K	Joback Method
tc	810.13	K	Joback Method
tf	304.85	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.11	J/mol×K	598.93	Joback Method
cpg	460.66	J/mol×K	634.13	Joback Method
cpg	476.24	J/mol×K	669.33	Joback Method
cpg	490.87	J/mol×K	704.53	Joback Method
cpg	504.59	J/mol×K	739.73	Joback Method
cpg	517.41	J/mol×K	774.93	Joback Method
cpg	529.36	J/mol×K	810.13	Joback Method
dvisc	0.0037379	Pa×s	304.85	Joback Method
dvisc	0.0014984	Pa×s	353.86	Joback Method

dvisc	0.0007503	Pa×s	402.88	Joback Method
dvisc	0.0004365	Pa×s	451.89	Joback Method
dvisc	0.0002824	Pa×s	500.90	Joback Method
dvisc	0.0001974	Pa×s	549.92	Joback Method
dvisc	0.0001463	Pa×s	598.93	Joback Method

Sources

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=U367942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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