Benzoic acid, 3-methyl-, 3-methylbut-2-yl ester

Inchi: InChI=1S/C13H18O2/c1-9(2)11(4)15-13(14)12-7-5-6-10(3)8-12/h5-9,11H,1-4H3
InchiKey: IVFWWWQYWNZVMP-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: Cc1cccc(C(=O)OC(C)C(C)C)c1
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	-77.44	kJ/mol	Joback Method
hf	-341.95	kJ/mol	Joback Method
hfus	18.82	kJ/mol	Joback Method
hvap	55.85	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.196		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinpol	1512.00		NIST Webbook
tb	603.91	K	Joback Method
tc	816.07	K	Joback Method
tf	317.37	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.86	J/mol×K	603.91	Joback Method
cpg	516.30	J/mol×K	780.71	Joback Method
cpg	503.59	J/mol×K	745.35	Joback Method
cpg	490.01	J/mol×K	709.99	Joback Method
cpg	475.54	J/mol×K	674.63	Joback Method
cpg	460.17	J/mol×K	639.27	Joback Method
cpg	528.17	J/mol×K	816.07	Joback Method
dvisc	0.0001436	Pa×s	603.91	Joback Method
dvisc	0.0001898	Pa×s	556.15	Joback Method

dvisc	0.0002643	Pa×s	508.40	Joback Method
dvisc	0.0003943	Pa×s	460.64	Joback Method
dvisc	0.0006450	Pa×s	412.88	Joback Method
dvisc	0.0012004	Pa×s	365.13	Joback Method
dvisc	0.0026930	Pa×s	317.37	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=U355705&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