4-Penten-2-ol, benzoate

Other names: 1-Methyl-3-butenyl benzoate
Inchi: InChI=1S/C12H14O2/c1-3-7-10(2)14-12(13)11-8-5-4-6-9-11/h3-6,8-10H,1,7H2,2H3
InchiKey: QLQPHDBTEQSJKE-UHFFFAOYSA-N
Formula: C12H14O2
SMILES: C=CCC(C)OC(=O)c1ccccc1
Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
gf	14.05	kJ/mol	Joback Method
hf	-179.13	kJ/mol	Joback Method
hfus	18.86	kJ/mol	Joback Method
hvap	52.68	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.808		Crippen Method
mcvol	159.320	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1380.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1374.00		NIST Webbook
ripol	1896.00		NIST Webbook
ripol	1911.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1896.00		NIST Webbook
ripol	1874.00		NIST Webbook

ripol	1876.00		NIST Webbook
ripol	1878.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1892.00		NIST Webbook
ripol	1892.00		NIST Webbook
ripol	1883.00		NIST Webbook
tb	573.17	K	Joback Method
tc	787.84	K	Joback Method
tf	306.82	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.17	J/mol×K	573.17	Joback Method
cpg	389.10	J/mol×K	608.95	Joback Method
cpg	403.11	J/mol×K	644.73	Joback Method
cpg	416.25	J/mol×K	680.50	Joback Method
cpg	428.53	J/mol×K	716.28	Joback Method
cpg	440.00	J/mol×K	752.06	Joback Method
cpg	450.68	J/mol×K	787.84	Joback Method
dvisc	0.0027806	Pa×s	306.82	Joback Method
dvisc	0.0013166	Pa×s	351.21	Joback Method
dvisc	0.0007373	Pa×s	395.60	Joback Method
dvisc	0.0004642	Pa×s	440.00	Joback Method
dvisc	0.0003181	Pa×s	484.39	Joback Method
dvisc	0.0002322	Pa×s	528.78	Joback Method
dvisc	0.0001780	Pa×s	573.17	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=R30965&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume