

3-Buten-1-ol, 3-methyl-, benzoate

Other names:	3-Methyl-3-butenyl benzoate 3-Methylbut-3-enyl benzoate
Inchi:	InChI=1S/C12H14O2/c1-10(2)8-9-14-12(13)11-6-4-3-5-7-11/h3-7H,1,8-9H2,2H3
InchiKey:	BBTRQSDRTFFNSW-UHFFFAOYSA-N
Formula:	C12H14O2
SMILES:	C=C(C)CCOC(=O)c1ccccc1
Mol. weight [g/mol]:	190.24
CAS:	5205-12-9

Physical Properties

Property code	Value	Unit	Source
gf	7.94	kJ/mol	Joback Method
hf	-183.64	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	53.15	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.810		Crippen Method
mcvol	159.320	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	1422.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1412.00		NIST Webbook
ripol	1993.00		NIST Webbook
ripol	1993.00		NIST Webbook
tb	573.49	K	Joback Method
tc	787.44	K	Joback Method
tf	307.86	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.59	J/mol×K	573.49	Joback Method
cpg	388.37	J/mol×K	609.15	Joback Method

cpg	402.26	J/mol×K	644.81	Joback Method
cpg	415.28	J/mol×K	680.46	Joback Method
cpg	427.48	J/mol×K	716.12	Joback Method
cpg	438.88	J/mol×K	751.78	Joback Method
cpg	449.51	J/mol×K	787.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5205129&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
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

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