

BENZOIC ACID, 3-METHYL-2-BUTENYL ESTER

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

Physical Properties

Property code	Value	Unit	Source
af	0.5084		Cheméo Relay (1.0)
gf	0.32	kJ/mol	Joback Method
hf	-261.36	kJ/mol	Cheméo Relay (1.0)
hfus	22.56	kJ/mol	Joback Method
hvap	71.16	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-3.78		Cheméo Relay (1.0)
logp	2.810		Crippen Method
mcvol	159.320	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1453.00		NIST Webbook
rinpol	1453.00		NIST Webbook
tb	535.01	K	Cheméo Relay (1.0)
tc	732.18	K	Cheméo Relay (1.0)
tf	268.79	K	Cheméo Relay (1.0)
vc	0.571	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.15	J/mol×K	580.97	Joback Method
cpg	389.04	J/mol×K	617.44	Joback Method
cpg	402.99	J/mol×K	653.92	Joback Method

cpg	416.04	J/mol×K	690.39	Joback Method
cpg	428.24	J/mol×K	726.86	Joback Method
cpg	439.62	J/mol×K	763.34	Joback Method
cpg	450.23	J/mol×K	799.81	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5205118&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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