

SEC-BUTYL BENZOATE

Other names:	1-Methylpropyl benzoate Sec-butyl benzoate
Inchi:	InChI=1S/C11H14O2/c1-3-9(2)13-11(12)10-7-5-4-6-8-10/h4-9H,3H2,1-2H3
InchiKey:	LSLWNAOQPPLHSW-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCC(C)OC(=O)c1ccccc1
Mol. weight [g/mol]:	178.23

Physical Properties

Property code	Value	Unit	Source
af	0.5206		Cheméo Relay (1.0)
gf	-82.21	kJ/mol	Joback Method
hf	-355.99	kJ/mol	Cheméo Relay (1.0)
hfus	17.55	kJ/mol	Joback Method
hvap	64.37	kJ/mol	Cheméo Relay (1.0)
ie	9.23	eV	Cheméo Relay (1.0)
log10ws	-3.05		Cheméo Relay (1.0)
logp	2.642		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1291.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1307.00		NIST Webbook
ripol	1749.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1752.00		NIST Webbook

ripol	1774.00		NIST Webbook
ripol	1766.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1792.00		NIST Webbook
ripol	1780.00		NIST Webbook
tb	505.53	K	Cheméo Relay (1.0)
tc	700.31	K	Cheméo Relay (1.0)
tf	239.20	K	Cheméo Relay (1.0)
vc	0.548	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.73	J/mol×K	553.61	Joback Method
cpg	423.32	J/mol×K	767.42	Joback Method
cpg	412.55	J/mol×K	731.79	Joback Method
cpg	401.00	J/mol×K	696.15	Joback Method
cpg	388.67	J/mol×K	660.52	Joback Method
cpg	375.53	J/mol×K	624.88	Joback Method
cpg	361.56	J/mol×K	589.25	Joback Method
dvisc	0.0004976	Pa×s	425.46	Joback Method
dvisc	0.0001883	Pa×s	553.61	Joback Method
dvisc	0.0002466	Pa×s	510.89	Joback Method
dvisc	0.0003393	Pa×s	468.18	Joback Method
dvisc	0.0030377	Pa×s	297.31	Joback Method
dvisc	0.0007949	Pa×s	382.74	Joback Method
dvisc	0.0014284	Pa×s	340.03	Joback Method

Sources

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=C3306363&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

af:	Acentric Factor
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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