

Butyl sorbate

Other names:	2,4-Hexadienoic acid, butyl ester, butyl (E,E)-hexa-2,4-dienoate
Inchi:	InChI=1S/C10H16O2/c1-3-5-7-8-10(11)12-9-6-4-2/h3,5,7-8H,4,6,9H2,1-2H3/b5-3+,8-7+
InchiKey:	SCVZKPKDMFXESQ-VSAQMIDASA-N
Formula:	C10H16O2
SMILES:	CC=CC=CC(=O)OCCCC
Mol. weight [g/mol]:	168.23
CAS:	7367-78-4

Physical Properties

Property code	Value	Unit	Source
gf	-40.16	kJ/mol	Joback Method
hf	-260.09	kJ/mol	Joback Method
hfus	24.85	kJ/mol	Joback Method
hvap	46.93	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.462		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1258.00		NIST Webbook
rinpol	1258.00		NIST Webbook
ripol	1694.00		NIST Webbook
ripol	1694.00		NIST Webbook
tb	512.81	K	Joback Method
tc	700.55	K	Joback Method
tf	264.46	K	Joback Method
vc	0.580	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.12	J/mol×K	512.81	Joback Method
cpg	346.55	J/mol×K	544.10	Joback Method
cpg	359.32	J/mol×K	575.39	Joback Method

cpg	371.48	J/molxK	606.68	Joback Method
cpg	383.03	J/molxK	637.97	Joback Method
cpg	394.01	J/molxK	669.26	Joback Method
cpg	404.45	J/molxK	700.55	Joback Method
dvisc	0.0028273	Paxs	264.46	Joback Method
dvisc	0.0012643	Paxs	305.85	Joback Method
dvisc	0.0006849	Paxs	347.24	Joback Method
dvisc	0.0004228	Paxs	388.63	Joback Method
dvisc	0.0002864	Paxs	430.03	Joback Method
dvisc	0.0002077	Paxs	471.42	Joback Method
dvisc	0.0001587	Paxs	512.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.00 ± 1.00	K	3.30	NIST Webbook

Sources

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=C7367784&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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