2-Butenoic acid, butyl ester

Other names:	Crotonic acid, butyl ester
	Butyl crotonate
	Butyl 2-butenoate
	(E)-2-Butenoic acid butyl ester
	Crotonic acid n-butyl ester
Inchi:	InChI=1S/C8H14O2/c1-3-5-7-10-8(9)6-4-2/h4,6H,3,5,7H2,1-2H3
InchiKey:	GWCTUKHUBWMAMI-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CC=CC(=O)OCCCC
Mol. weight [g/mol]:	142.20
CAS:	7299-91-4

Physical Properties

Property code	Value	Unit	Source
chl	-4681.10 ± 2.90	kJ/mol	NIST Webbook
gf	-137.22	kJ/mol	Joback Method
hf	-416.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-468.00 ± 3.00	kJ/mol	NIST Webbook
hfus	19.46	kJ/mol	Joback Method
hvap	52.00	kJ/mol	NIST Webbook
hvap	52.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-1.89		Crippen Method
logp	1.906		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
rinpol	1027.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1024.00		NIST Webbook

ripol	1332.00		NIST Webbook
ripol	1334.00		NIST Webbook
tb	462.89	K	Joback Method
tc	646.21	K	Joback Method
tf	247.00	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.30	J/mol×K	462.89	Joback Method
cpg	317.95	J/mol×K	615.66	Joback Method
cpg	307.96	J/mol×K	585.10	Joback Method
cpg	297.52	J/mol×K	554.55	Joback Method
cpg	286.60	J/mol×K	524.00	Joback Method
cpg	275.19	J/mol×K	493.44	Joback Method
cpg	327.49	J/mol×K	646.21	Joback Method
dvisc	0.0002123	Pa×s	462.89	Joback Method
dvisc	0.0002744	Pa×s	426.91	Joback Method
dvisc	0.0003717	Pa×s	390.93	Joback Method
dvisc	0.0005355	Pa×s	354.94	Joback Method
dvisc	0.0008378	Pa×s	318.96	Joback Method
dvisc	0.0014687	Pa×s	282.98	Joback Method
dvisc	0.0030324	Pa×s	247.00	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7299914&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

chl: Standard liquid enthalpy of combustion

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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