Isopentyl 2-butenoate

Other names: 2-Butenoic acid, 3-methyl, butyl ester
Isopentyl 2-butenoate
(E)-2-Butenoic acid 3-methylbutyl ester
Inchi: InChI=1S/C9H16O2/c1-4-5-9(10)11-7-6-8(2)3/h4-5,8H,6-7H2,1-3H3
InchiKey: JAVOYFHBJFLMRQ-SNAWJCMRSA-N
Formula: C9H16O2
SMILES: C/C=C/C(=O)OCCC(C)C
Mol. weight [g/mol]: 156.23

Physical Properties

Property code	Value	Unit	Source
chl	-5327.50 ± 2.90	kJ/mol	NIST Webbook
hf	-447.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-501.00 ± 3.00	kJ/mol	NIST Webbook
hfus	18.53	kJ/mol	Joback Method
hvap	54.00	kJ/mol	NIST Webbook
hvap	54.00 ± 1.00	kJ/mol	NIST Webbook
ie	9.78	eV	Cheméo Relay (1.0)
log10ws	-3.10		Cheméo Relay (1.0)
logp	2.152		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1082.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1088.00		NIST Webbook
tb	450.59	K	Cheméo Relay (1.0)
tc	646.24	K	Cheméo Relay (1.0)
tf	205.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	306.21	J/mol×K	485.33	Joback Method
cpg	319.47	J/mol×K	516.24	Joback Method
cpg	332.17	J/mol×K	547.14	Joback Method
cpg	344.30	J/mol×K	578.05	Joback Method
cpg	355.88	J/mol×K	608.96	Joback Method
cpg	366.93	J/mol×K	639.87	Joback Method
cpg	377.46	J/mol×K	670.77	Joback Method
dvisc	0.0044834	Pa×s	243.27	Joback Method
dvisc	0.0018217	Pa×s	283.61	Joback Method
dvisc	0.0009263	Pa×s	323.96	Joback Method
dvisc	0.0005471	Pa×s	364.30	Joback Method
dvisc	0.0003589	Pa×s	404.64	Joback Method
dvisc	0.0002542	Pa×s	444.99	Joback Method
dvisc	0.0001906	Pa×s	485.33	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25415774&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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

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