Pentyl 3-butenoate

Other names:	3-Butenoic acid, pentyl ester
Inchi:	InChI=1S/C9H16O2/c1-3-5-6-8-11-9(10)7-4-2/h4H,2-3,5-8H2,1H3
InchiKey:	BUSVERZYRXOWCB-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	C=CCC(=O)OCCCCC
Mol. weight [g/mol]:	156.22

Physical Properties

Property code	Value	Unit	Source
gf	-121.18	kJ/mol	Joback Method
hf	-348.46	kJ/mol	Joback Method
hfus	20.57	kJ/mol	Joback Method
hvap	44.11	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1049.00		NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1065.00		NIST Webbook
tb	478.29	K	Joback Method
tc	655.34	K	Joback Method
tf	261.59	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.44	J/mol×K	478.29	Joback Method
cpg	318.12	J/mol×K	507.80	Joback Method
cpg	330.31	J/mol×K	537.31	Joback Method
cpg	342.00	J/mol×K	566.81	Joback Method
cpg	353.22	J/mol×K	596.32	Joback Method
cpg	363.97	J/mol×K	625.83	Joback Method

cpg	374.26	J/mol×K	655.34	Joback Method
dvisc	0.0030378	Pa×s	261.59	Joback Method
dvisc	0.0015428	Pa×s	297.71	Joback Method
dvisc	0.0009072	Pa×s	333.82	Joback Method
dvisc	0.0005918	Pa×s	369.94	Joback Method
dvisc	0.0004165	Pa×s	406.06	Joback Method
dvisc	0.0003104	Pa×s	442.17	Joback Method
dvisc	0.0002419	Pa×s	478.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R5386&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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