4-Penten-1-ol, propanoate

Other names:	4-Pentenyl propionate
	Propanoic acid, 4-pentenyl ester
Inchi:	InChI=1S/C8H14O2/c1-3-5-6-7-10-8(9)4-2/h3H,1,4-7H2,2H3
InchiKey:	ROJSQZUHNAFOPE-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	C=CCCCOC(=O)CC
Mol. weight [g/mol]:	142.20
CAS:	30563-30-5

Physical Properties

Property code	Value	Unit	Source
gf	-129.60	kJ/mol	Joback Method
hf	-327.82	kJ/mol	Joback Method
hfus	17.98	kJ/mol	Joback Method
hvap	41.89	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.906		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	958.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	986.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1300.00		NIST Webbook
tb	455.41	K	Joback Method
tc	633.98	K	Joback Method
tf	250.32	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.07	J/mol×K	455.41	Joback Method
cpg	274.71	J/mol×K	485.17	Joback Method
cpg	285.90	J/mol×K	514.93	Joback Method
cpg	296.66	J/mol×K	544.69	Joback Method
cpg	306.99	J/mol×K	574.46	Joback Method
cpg	316.89	J/mol×K	604.22	Joback Method
cpg	326.37	J/mol×K	633.98	Joback Method
dvisc	0.0029783	Pa×s	250.32	Joback Method
dvisc	0.0015454	Pa×s	284.50	Joback Method
dvisc	0.0009231	Pa×s	318.68	Joback Method
dvisc	0.0006093	Pa×s	352.87	Joback Method
dvisc	0.0004328	Pa×s	387.05	Joback Method
dvisc	0.0003249	Pa×s	421.23	Joback Method
dvisc	0.0002547	Pa×s	455.41	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30563305&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

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