2-Butenoic acid, pentyl ester

Other names: amyl crotonate
pentyl 2-butenoate
Inchi: InChI=1S/C9H16O2/c1-3-5-6-8-11-9(10)7-4-2/h4,7H,3,5-6,8H2,1-2H3/b7-4+
InchiKey: PWYYERNADDIMJR-QPJJXVBHSA-N
Formula: C9H16O2
SMILES: CC=CC(=O)OCCCCC
Mol. weight [g/mol]: 156.22
CAS: 25415-76-3

Physical Properties

Property code	Value	Unit	Source
gf	-128.80	kJ/mol	Joback Method
hf	-356.67	kJ/mol	Joback Method
hfus	22.05	kJ/mol	Joback Method
hvap	44.74	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	1110.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1119.00		NIST Webbook
tb	485.77	K	Joback Method
tc	667.32	K	Joback Method
tf	258.27	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.02	J/mol×K	485.77	Joback Method
cpg	365.29	J/mol×K	637.06	Joback Method
cpg	354.47	J/mol×K	606.80	Joback Method

cpg	343.15	J/mol×K	576.54	Joback Method
cpg	331.30	J/mol×K	546.29	Joback Method
cpg	318.93	J/mol×K	516.03	Joback Method
cpg	375.62	J/mol×K	667.32	Joback Method
dvisc	0.0002011	Pa×s	485.77	Joback Method
dvisc	0.0002612	Pa×s	447.85	Joback Method
dvisc	0.0003563	Pa×s	409.94	Joback Method
dvisc	0.0005177	Pa×s	372.02	Joback Method
dvisc	0.0008186	Pa×s	334.10	Joback Method
dvisc	0.0014558	Pa×s	296.19	Joback Method
dvisc	0.0030655	Pa×s	258.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25415763&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

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