Butanoic acid, 4-pentenyl ester

Inchi: InChI=1S/C9H16O2/c1-3-5-6-8-11-9(10)7-4-2/h3H,1,4-8H2,2H3
InchiKey: DTGXDHGNUDOWJS-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: C=CCCCOC(=O)CCC
Mol. weight [g/mol]: 156.22
CAS: 30563-31-6

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	1070.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1070.00		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	363.97	J/mol×K	625.83	Joback Method
cpg	353.22	J/mol×K	596.32	Joback Method
cpg	342.00	J/mol×K	566.81	Joback Method

cpg	330.31	J/mol×K	537.31	Joback Method
cpg	318.12	J/mol×K	507.80	Joback Method
cpg	374.26	J/mol×K	655.34	Joback Method
dvisc	0.0002419	Pa×s	478.29	Joback Method
dvisc	0.0003104	Pa×s	442.17	Joback Method
dvisc	0.0004165	Pa×s	406.06	Joback Method
dvisc	0.0005918	Pa×s	369.94	Joback Method
dvisc	0.0009072	Pa×s	333.82	Joback Method
dvisc	0.0015428	Pa×s	297.71	Joback Method
dvisc	0.0030378	Pa×s	261.59	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30563316&Units=SI

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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