2-Pentenoic acid butyl ester

Inchi: InChI=1S/C9H16O2/c1-3-5-7-9(10)11-8-6-4-2/h5,7H,3-4,6,8H2,1-2H3/b7-5+
InchiKey: URYUTJWQTWWCCN-FNORWQNLSA-N
Formula: C9H16O2
SMILES: CCC=CC(=O)OCCCC
Mol. weight [g/mol]: 156.22
CAS: 79947-84-5

Physical Properties

Property code	Value	Unit	Source
chl	-5333.30 ± 2.50	kJ/mol	NIST Webbook
gf	-128.80	kJ/mol	Joback Method
hf	-440.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-495.00 ± 3.00	kJ/mol	NIST Webbook
hfus	22.05	kJ/mol	Joback Method
hvap	55.00 ± 1.00	kJ/mol	NIST Webbook
hvap	55.00	kJ/mol	NIST Webbook
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
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	318.93	J/mol×K	516.03	Joback Method
cpg	331.30	J/mol×K	546.29	Joback Method
cpg	343.15	J/mol×K	576.54	Joback Method
cpg	354.47	J/mol×K	606.80	Joback Method
cpg	365.29	J/mol×K	637.06	Joback Method

cpg	375.62	J/mol×K	667.32	Joback Method
dvisc	0.0030655	Pa×s	258.27	Joback Method
dvisc	0.0014558	Pa×s	296.19	Joback Method
dvisc	0.0008186	Pa×s	334.10	Joback Method
dvisc	0.0005177	Pa×s	372.02	Joback Method
dvisc	0.0003563	Pa×s	409.94	Joback Method
dvisc	0.0002612	Pa×s	447.85	Joback Method
dvisc	0.0002011	Pa×s	485.77	Joback Method
hvapt	43.50	kJ/mol	293.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C79947845&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

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
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
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume