Pentanoic acid, 1,1-dimethylethyl ester

Inchi: InChI=1S/C9H18O2/c1-5-6-7-8(10)11-9(2,3)4/h5-7H2,1-4H3
InchiKey: SCSLUABEVMLYEA-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCCCC(=O)OC(C)(C)C
Mol. weight [g/mol]: 158.24
CAS: 23361-78-6

Physical Properties

Property code	Value	Unit	Source
gf	-206.18	kJ/mol	Joback Method
hf	-482.64	kJ/mol	Joback Method
hfus	14.44	kJ/mol	Joback Method
hvap	43.49	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.518		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	957.00		NIST Webbook
rinpol	957.00		NIST Webbook
ripol	1135.00		NIST Webbook
ripol	1135.00		NIST Webbook
tb	478.38	K	Joback Method
tc	662.57	K	Joback Method
tf	265.77	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.67	J/mol×K	478.38	Joback Method
cpg	340.03	J/mol×K	509.08	Joback Method
cpg	353.74	J/mol×K	539.78	Joback Method
cpg	366.81	J/mol×K	570.48	Joback Method
cpg	379.26	J/mol×K	601.18	Joback Method

cpg	391.10	J/mol×K	631.87	Joback Method
cpg	402.36	J/mol×K	662.57	Joback Method
dvisc	0.0045510	Pa×s	265.77	Joback Method
dvisc	0.0020820	Pa×s	301.20	Joback Method
dvisc	0.0011229	Pa×s	336.64	Joback Method
dvisc	0.0006812	Pa×s	372.07	Joback Method
dvisc	0.0004508	Pa×s	407.51	Joback Method
dvisc	0.0003187	Pa×s	442.94	Joback Method
dvisc	0.0002372	Pa×s	478.38	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23361786&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from: