4-Pentenal, 2-ethyl-

Other names: 2-Ethyl-4-pentenal
Inchi: InChI=1S/C7H12O/c1-3-5-7(4-2)6-8/h3,6-7H,1,4-5H2,2H3
InchiKey: UADJTDURPOSPRM-UHFFFAOYSA-N
Formula: C7H12O
SMILES: C=CCC(C=O)CC
Mol. weight [g/mol]: 112.17
CAS: 5204-80-8

Physical Properties

Property code	Value	Unit	Source
gf	-6.06	kJ/mol	Joback Method
hf	-153.24	kJ/mol	Joback Method
hfus	11.37	kJ/mol	Joback Method
hvap	36.84	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.788		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
rinpol	1034.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1034.00		NIST Webbook
tb	404.46	K	Joback Method
tc	583.78	K	Joback Method
tf	193.89	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.97	J/mol×K	404.46	Joback Method
cpg	212.72	J/mol×K	434.35	Joback Method
cpg	223.00	J/mol×K	464.23	Joback Method
cpg	232.82	J/mol×K	494.12	Joback Method
cpg	242.20	J/mol×K	524.01	Joback Method

cpg	251.15	J/mol×K	553.89	Joback Method
cpg	259.69	J/mol×K	583.78	Joback Method
dvisc	0.0063907	Pa×s	193.89	Joback Method
dvisc	0.0026059	Pa×s	228.98	Joback Method
dvisc	0.0013487	Pa×s	264.08	Joback Method
dvisc	0.0008147	Pa×s	299.17	Joback Method
dvisc	0.0005471	Pa×s	334.27	Joback Method
dvisc	0.0003962	Pa×s	369.37	Joback Method
dvisc	0.0003035	Pa×s	404.46	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=C5204808&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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