2-Pentenal, isomer 2

Inchi: InChI=1S/C5H8O/c1-2-3-4-5-6/h3-5H,2H2,1H3
InchiKey: DTCCTIQRPGSLPT-UHFFFAOYSA-N
Formula: C5H8O
SMILES: CCC=CC=O
Mol. weight [g/mol]: 84.12

Physical Properties

Property code	Value	Unit	Source
gf	-28.08	kJ/mol	Joback Method
hf	-114.89	kJ/mol	Joback Method
hfus	11.20	kJ/mol	Joback Method
hvap	33.40	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.151		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
ripol	1145.00		NIST Webbook
tb	366.62	K	Joback Method
tc	548.86	K	Joback Method
tf	183.03	K	Joback Method
vc	0.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.02	J/mol×K	366.62	Joback Method
cpg	138.10	J/mol×K	396.99	Joback Method
cpg	145.79	J/mol×K	427.37	Joback Method
cpg	153.10	J/mol×K	457.74	Joback Method
cpg	160.05	J/mol×K	488.11	Joback Method
cpg	166.65	J/mol×K	518.49	Joback Method
cpg	172.92	J/mol×K	548.86	Joback Method
dvisc	0.0033669	Pa×s	183.03	Joback Method
dvisc	0.0016007	Pa×s	213.63	Joback Method

dvisc	0.0009169	Pa×s	244.23	Joback Method
dvisc	0.0005946	Pa×s	274.82	Joback Method
dvisc	0.0004205	Pa×s	305.42	Joback Method
dvisc	0.0003168	Pa×s	336.02	Joback Method
dvisc	0.0002502	Pa×s	366.62	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=R613771&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume