(E)-3-Heptenal

Inchi: InChI=1S/C6H10O/c1-2-3-4-5-6-7/h3-4,6H,2,5H2,1H3/b4-3+
InchiKey: GXANMBISFKBPEX-ONEGZZNKSA-N
Formula: C6H10O
SMILES: CCC=CCC=O
Mol. weight [g/mol]: 98.14

Physical Properties

Property code	Value	Unit	Source
gf	-19.66	kJ/mol	Joback Method
hf	-135.53	kJ/mol	Joback Method
hfus	13.79	kJ/mol	Joback Method
hvap	35.63	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	877.00		NIST Webbook
rinpol	957.00		NIST Webbook
tb	389.50	K	Joback Method
tc	570.95	K	Joback Method
tf	194.30	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.69	J/mol×K	389.50	Joback Method
cpg	174.16	J/mol×K	419.74	Joback Method
cpg	183.18	J/mol×K	449.98	Joback Method
cpg	191.76	J/mol×K	480.23	Joback Method
cpg	199.93	J/mol×K	510.47	Joback Method
cpg	207.70	J/mol×K	540.71	Joback Method
cpg	215.09	J/mol×K	570.95	Joback Method
dvisc	0.0038680	Pa×s	194.30	Joback Method

dvisc	0.0017894	Pa×s	226.83	Joback Method
dvisc	0.0010044	Pa×s	259.37	Joback Method
dvisc	0.0006413	Pa×s	291.90	Joback Method
dvisc	0.0004480	Pa×s	324.43	Joback Method
dvisc	0.0003341	Pa×s	356.97	Joback Method
dvisc	0.0002617	Pa×s	389.50	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=R626549&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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