Heptanal, 2-methyl-

Other names: 2-Methylheptanal
2-methylheptan-1-al
Inchi: InChI=1S/C8H16O/c1-3-4-5-6-8(2)7-9/h7-8H,3-6H2,1-2H3
InchiKey: DHEKCFIOOSCJRW-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CCCCCC(C)C=O
Mol. weight [g/mol]: 128.21
CAS: 16630-91-4

Physical Properties

Property code	Value	Unit	Source
gf	-85.48	kJ/mol	Joback Method
hf	-299.31	kJ/mol	Joback Method
hfus	15.24	kJ/mol	Joback Method
hvap	39.73	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.402		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
ripol	1306.00		NIST Webbook
ripol	1306.00		NIST Webbook
tb	430.66	K	Joback Method
tc	605.22	K	Joback Method
tf	206.92	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.75	J/mol×K	430.66	Joback Method
cpg	269.26	J/mol×K	459.75	Joback Method
cpg	281.26	J/mol×K	488.85	Joback Method
cpg	292.77	J/mol×K	517.94	Joback Method
cpg	303.81	J/mol×K	547.04	Joback Method

cpg	314.39	J/mol×K	576.13	Joback Method
cpg	324.51	J/mol×K	605.22	Joback Method
dvisc	0.0077983	Pa×s	206.92	Joback Method
dvisc	0.0030008	Pa×s	244.21	Joback Method
dvisc	0.0014872	Pa×s	281.50	Joback Method
dvisc	0.0008686	Pa×s	318.79	Joback Method
dvisc	0.0005678	Pa×s	356.08	Joback Method
dvisc	0.0004023	Pa×s	393.37	Joback Method
dvisc	0.0003026	Pa×s	430.66	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51993e+01
Coeff. B	-4.00408e+03
Coeff. C	-6.24000e+01
Temperature range (K), min.	330.92
Temperature range (K), max.	467.35

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16630914&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume