

2-Heptenal, 2-methyl-

Other names:	(E)-2-Methyl-2-heptenal 2-methyl-2-heptenal
Inchi:	InChI=1S/C8H14O/c1-3-4-5-6-8(2)7-9/h6-7H,3-5H2,1-2H3/b8-6+
InchiKey:	IGNVJMUTQIKSHB-SOFGYWHQSA-N
Formula:	C8H14O
SMILES:	CCCCC=C(C)C=O
Mol. weight [g/mol]:	126.20
CAS:	30567-26-1

Physical Properties

Property code	Value	Unit	Source
gf	-11.37	kJ/mol	Joback Method
hf	-186.60	kJ/mol	Joback Method
hfus	17.66	kJ/mol	Joback Method
hvap	40.16	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mvol	120.850	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
ripol	1342.00		NIST Webbook
tb	435.14	K	Joback Method
tc	617.65	K	Joback Method
tf	202.88	K	Joback Method
vc	0.481	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.01	J/mol×K	435.14	Joback Method
cpg	253.06	J/mol×K	465.56	Joback Method
cpg	264.55	J/mol×K	495.98	Joback Method
cpg	275.48	J/mol×K	526.39	Joback Method
cpg	285.90	J/mol×K	556.81	Joback Method
cpg	295.81	J/mol×K	587.23	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42785e+01
Coeff. B	-3.78183e+03
Coeff. C	-6.60140e+01
Temperature range (K), min.	336.32
Temperature range (K), max.	487.76

Sources

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=C30567261&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/ci9903071>

Legend

cpg:	Ideal gas heat capacity
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
mccvol:	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

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