

3-Heptene, 4-propyl-

Other names:	4-Propyl-3-heptene
Inchi:	InChI=1S/C10H20/c1-4-7-10(8-5-2)9-6-3/h7H,4-6,8-9H2,1-3H3
InchiKey:	JEVSSCXTVQHWCX-UHFFFAOYSA-N
Formula:	C10H20
SMILES:	CCC=C(CCC)CCC
Mol. weight [g/mol]:	140.27
CAS:	4485-13-6

Physical Properties

Property code	Value	Unit	Source
gf	104.99	kJ/mol	Joback Method
hf	-142.30	kJ/mol	Joback Method
hfus	20.55	kJ/mol	Joback Method
hvap	37.89	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.923		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
tb	432.24	K	Joback Method
tc	605.63	K	Joback Method
tf	183.42	K	Joback Method
vc	0.577	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.23	J/mol×K	432.24	Joback Method
cpg	315.43	J/mol×K	461.14	Joback Method
cpg	329.98	J/mol×K	490.04	Joback Method
cpg	343.91	J/mol×K	518.94	Joback Method
cpg	357.23	J/mol×K	547.83	Joback Method
cpg	369.97	J/mol×K	576.73	Joback Method
cpg	382.16	J/mol×K	605.63	Joback Method
hvapt	43.70	kJ/mol	352.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50344e+01
Coeff. B	-3.87422e+03
Coeff. C	-6.17050e+01
Temperature range (K), min.	324.42
Temperature range (K), max.	460.17

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	https://webbook.nist.gov/cgi/cbook.cgi?ID=C4485136&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/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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