

Octane, 4-propyl-

Other names:	4-propyloctane
Inchi:	InChI=1S/C11H24/c1-4-7-10-11(8-5-2)9-6-3/h11H,4-10H2,1-3H3
InchiKey:	VFAMBAFLNKONTN-UHFFFAOYSA-N
Formula:	C11H24
SMILES:	CCCCC(CCC)CCC
Mol. weight [g/mol]:	156.31
CAS:	17302-13-5

Physical Properties

Property code	Value	Unit	Source
gf	39.30	kJ/mol	Joback Method
hf	-275.65	kJ/mol	Joback Method
hfus	20.72	kJ/mol	Joback Method
hvap	39.69	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.393		Crippen Method
mcvol	165.850	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
tb	450.64	K	Joback Method
tc	615.77	K	Joback Method
tf	198.73	K	Joback Method
vc	0.645	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.10	J/mol×K	450.64	Joback Method
cpg	376.48	J/mol×K	478.16	Joback Method
cpg	392.24	J/mol×K	505.68	Joback Method
cpg	407.41	J/mol×K	533.20	Joback Method
cpg	421.98	J/mol×K	560.73	Joback Method
cpg	435.99	J/mol×K	588.25	Joback Method
cpg	449.44	J/mol×K	615.77	Joback Method
dvisc	0.0105797	Paxs	198.73	Joback Method

dvisc	0.0031400	Paxs	240.72	Joback Method
dvisc	0.0013369	Paxs	282.70	Joback Method
dvisc	0.0007098	Paxs	324.69	Joback Method
dvisc	0.0004357	Paxs	366.67	Joback Method
dvisc	0.0002956	Paxs	408.65	Joback Method
dvisc	0.0002156	Paxs	450.64	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41201e+01
Coeff. B	-3.49380e+03
Coeff. C	-8.54500e+01
Temperature range (K), min.	338.03
Temperature range (K), max.	482.08

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=C17302135&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cp_g:	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
h_{vap}:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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