3-Heptyne

Other names: 1-ETHYL-2-PROPYLACETYLENE
hept-3-yne
Inchi: InChI=1S/C7H12/c1-3-5-7-6-4-2/h3-5H2,1-2H3
InchiKey: KLYHSJRCIZOUHE-UHFFFAOYSA-N
Formula: C7H12
SMILES: CCC#CCCC
Mol. weight [g/mol]: 96.17
CAS: 2586-89-2

Physical Properties

Property code	Value	Unit	Source
gf	210.86	kJ/mol	Joback Method
hf	82.80 ± 2.40	kJ/mol	NIST Webbook
hfus	17.01	kJ/mol	Joback Method
hvap	33.33	kJ/mol	Joback Method
ie	9.26 ± 0.01	eV	NIST Webbook
log10ws	-2.55		Crippen Method
logp	2.200		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
rinpol	717.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	716.00		NIST Webbook
rinpol	716.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	744.00		NIST Webbook
ripol	913.00		NIST Webbook

ripol	916.00		NIST Webbook
ripol	926.10		NIST Webbook
ripol	910.00		NIST Webbook
tb	379.00 ± 2.00	K	NIST Webbook
tb	379.65 ± 2.00	K	NIST Webbook
tb	380.40	K	NIST Webbook
tb	380.31 ± 0.30	K	NIST Webbook
tb	378.50 ± 0.50	K	NIST Webbook
tc	556.83	K	Joback Method
tf	170.00 ± 2.00	K	NIST Webbook
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.10	J/mol×K	525.45	Joback Method
cpg	171.96	J/mol×K	368.56	Joback Method
cpg	182.57	J/mol×K	399.94	Joback Method
cpg	192.78	J/mol×K	431.32	Joback Method
cpg	202.60	J/mol×K	462.70	Joback Method
cpg	212.03	J/mol×K	494.08	Joback Method
cpg	229.80	J/mol×K	556.83	Joback Method
hvapt	39.10	kJ/mol	361.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39016e+01
Coeff. B	-2.98598e+03
Coeff. C	-5.86580e+01
Temperature range (K), min.	277.99
Temperature range (K), max.	406.26

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.19322e+01
Coeff. B	-8.01335e+03
Coeff. C	-1.13473e+01
Coeff. D	8.14992e-06
Temperature range (K), min.	343.15
Temperature range (K), max.	380.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol416.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2586892&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=416
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume