3,5-Octadiyne

Other names: Diethyldiacetylene
Inchi: InChI=1S/C8H10/c1-3-5-7-8-6-4-2/h3-4H2,1-2H3
InchiKey: LILZEAJBVQOINI-UHFFFAOYSA-N
Formula: C8H10
SMILES: CCC#CC#CCC
Mol. weight [g/mol]: 106.17
CAS: 16387-70-5

Physical Properties

Property code	Value	Unit	Source
gf	422.08	kJ/mol	Joback Method
hf	336.15	kJ/mol	Joback Method
hfus	22.72	kJ/mol	Joback Method
hvap	37.71	kJ/mol	Joback Method
ie	8.78	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
ie	8.55	eV	NIST Webbook
log10ws	-2.76		Crippen Method
logp	1.813		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
rinpol	972.00		NIST Webbook
tb	437.00 ± 4.00	K	NIST Webbook
tc	616.12	K	Joback Method
tf	392.12	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.91	J/mol×K	400.44	Joback Method
cpg	193.56	J/mol×K	436.39	Joback Method
cpg	203.76	J/mol×K	472.33	Joback Method
cpg	213.53	J/mol×K	508.28	Joback Method

cpg	222.88	J/mol×K	544.23	Joback Method
cpg	231.82	J/mol×K	580.18	Joback Method
cpg	240.36	J/mol×K	616.12	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62366e+01
Coeff. B	-4.35058e+03
Coeff. C	-6.25390e+01
Temperature range (K), min.	335.32
Temperature range (K), max.	460.76

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=C16387705&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

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