5-Decyne

Other names: 1,2-Dibutylacetylene
5-C10H18
Dibutylacetylene
Inchi: InChI=1S/C10H18/c1-3-5-7-9-10-8-6-4-2/h3-8H2,1-2H3
InchiKey: JWBQJUFCNOLNNC-UHFFFAOYSA-N
Formula: C10H18
SMILES: CCCCC#CCCCC
Mol. weight [g/mol]: 138.25
CAS: 1942-46-7

Physical Properties

Property code	Value	Unit	Source
gf	236.12	kJ/mol	Joback Method
hf	18.70 ± 3.30	kJ/mol	NIST Webbook
hfus	24.78	kJ/mol	Joback Method
hvap	40.01	kJ/mol	Joback Method
ie	9.14 ± 0.02	eV	NIST Webbook
ie	9.12 ± 0.01	eV	NIST Webbook
log10ws	-3.80		Crippen Method
logp	3.370		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1008.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1008.00		NIST Webbook
ripol	1191.00		NIST Webbook
ripol	1171.00		NIST Webbook
ripol	1182.70		NIST Webbook
ripol	1168.40		NIST Webbook
ripol	1186.10		NIST Webbook

ripol	1191.00		NIST Webbook
ripol	1191.00		NIST Webbook
ripol	1191.00		NIST Webbook
ripol	1188.10		NIST Webbook
ripol	1190.00		NIST Webbook
tb	453.00 ± 3.00	K	NIST Webbook
tc	621.64	K	Joback Method
tf	200.00 ± 1.50	K	NIST Webbook
tf	196.00 ± 3.00	K	NIST Webbook
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.31	J/mol×K	437.20	Joback Method
cpg	302.76	J/mol×K	467.94	Joback Method
cpg	316.63	J/mol×K	498.68	Joback Method
cpg	329.93	J/mol×K	529.42	Joback Method
cpg	342.68	J/mol×K	560.16	Joback Method
cpg	354.90	J/mol×K	590.90	Joback Method
cpg	366.61	J/mol×K	621.64	Joback Method
hvapt	45.50	kJ/mol	482.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	450.00	K	100.00	NIST Webbook
tbrp	373.00	K	11.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53961e+01

Coeff. B	-4.13713e+03
Coeff. C	-6.62920e+01
Temperature range (K), min.	340.12
Temperature range (K), max.	476.53

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1942467&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume