3-Decyne

Other names: 3-C10H18
Inchi: InChI=1S/C10H18/c1-3-5-7-9-10-8-6-4-2/h3-5,7,9-10H2,1-2H3
InchiKey: JUWXVJKQNKKRLD-UHFFFAOYSA-N
Formula: C10H18
SMILES: CCC#CCCCCCC
Mol. weight [g/mol]: 138.25
CAS: 2384-85-2

Physical Properties

Property code	Value	Unit	Source
gf	236.12	kJ/mol	Joback Method
hf	21.80 ± 3.30	kJ/mol	NIST Webbook
hfus	24.78	kJ/mol	Joback Method
hvap	40.01	kJ/mol	Joback Method
ie	9.19 ± 0.02	eV	NIST Webbook
ie	9.19 ± 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	1019.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1017.00		NIST Webbook
ripol	1190.30		NIST Webbook
ripol	1208.00		NIST Webbook
ripol	1185.30		NIST Webbook
ripol	1197.50		NIST Webbook
ripol	1187.50		NIST Webbook
ripol	1202.70		NIST Webbook
ripol	1203.10		NIST Webbook

ripol	1207.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1199.20		NIST Webbook
ripol	1196.20		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1207.00		NIST Webbook
tb	176.00 ± 2.00	K	NIST Webbook
tb	448.65 ± 1.50	K	NIST Webbook
tc	621.64	K	Joback Method
tf	308.56	K	Joback Method
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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53983e+01
Coeff. B	-4.15588e+03
Coeff. C	-6.69310e+01
Temperature range (K), min.	341.96
Temperature range (K), max.	478.94

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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol437.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2384852&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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