1-Tetradecyne

Other names: 1-C14H26
tetradecyne
Inchi: InChI=1S/C14H26/c1-3-5-7-9-11-13-14-12-10-8-6-4-2/h1H,4-14H2,2H3
InchiKey: DZEFNRWGWQDGTR-UHFFFAOYSA-N
Formula: C14H26
SMILES: C#CCCCCCCCCCCCC
Mol. weight [g/mol]: 194.36
CAS: 765-10-6

Physical Properties

Property code	Value	Unit	Source
af	0.5910		KDB
gf	290.07	kJ/mol	Joback Method
hf	-40.39	kJ/mol	Joback Method
hfus	34.99	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
ie	9.89 ± 0.02	eV	NIST Webbook
log10ws	-5.48		Crippen Method
logp	4.931		Crippen Method
mcvol	199.520	ml/mol	McGowan Method
pc	1720.00	kPa	KDB
rinpol	1398.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1413.00		NIST Webbook
ripol	1603.50		NIST Webbook
ripol	1626.20		NIST Webbook
ripol	1633.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1633.00		NIST Webbook
ripol	1633.00		NIST Webbook
ripol	1633.00		NIST Webbook
ripol	1627.40		NIST Webbook
ripol	1626.20		NIST Webbook
ripol	1603.50		NIST Webbook
ripol	1603.50		NIST Webbook

ripol	1633.00		NIST Webbook
tb	525.20	K	KDB
tc	698.90	K	KDB
tf	273.00	K	KDB
vc	0.781	m3/kmol	KDB
zc	0.2313160		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.41	J/mol×K	509.84	Joback Method
cpg	485.68	J/mol×K	537.96	Joback Method
cpg	502.24	J/mol×K	566.07	Joback Method
cpg	518.10	J/mol×K	594.19	Joback Method
cpg	533.29	J/mol×K	622.31	Joback Method
cpg	547.83	J/mol×K	650.43	Joback Method
cpg	561.75	J/mol×K	678.54	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	406.00 ± 1.00	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55614e+01
Coeff. B	-4.78036e+03
Coeff. C	-8.71420e+01
Temperature range (K), min.	400.12
Temperature range (K), max.	553.52

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.89402e+01
Coeff. B	-1.06623e+04
Coeff. C	-1.03762e+01
Coeff. D	3.53458e-06
Temperature range (K), min.	438.00
Temperature range (K), max.	619.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C765106&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=439
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/mol439.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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

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