7-Tetradecyne

Other names: 7-C14H26
7-Tetadecyne
Inchi: InChI=1S/C14H26/c1-3-5-7-9-11-13-14-12-10-8-6-4-2/h3-12H2,1-2H3
InchiKey: AFNWSIIBAYUTTL-UHFFFAOYSA-N
Formula: C14H26
SMILES: CCCCCCC#CCCCCCC
Mol. weight [g/mol]: 194.36
CAS: 35216-11-6

Physical Properties

Property code	Value	Unit	Source
gf	269.80	kJ/mol	Joback Method
hf	-59.99	kJ/mol	Joback Method
hfus	35.14	kJ/mol	Joback Method
hvap	48.91	kJ/mol	Joback Method
ie	9.03 ± 0.04	eV	NIST Webbook
ie	9.07 ± 0.01	eV	NIST Webbook
log10ws	-5.48		Crippen Method
logp	4.931		Crippen Method
mcvol	199.520	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1416.00		NIST Webbook
ripol	1562.30		NIST Webbook
ripol	1562.30		NIST Webbook
ripol	1545.10		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1545.10		NIST Webbook
ripol	1562.30		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1572.00		NIST Webbook
ripol	1572.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1574.00		NIST Webbook

ripol	1575.00		NIST Webbook
ripol	1541.30		NIST Webbook
ripol	1545.10		NIST Webbook
tb	528.72	K	Joback Method
tc	706.35	K	Joback Method
tf	353.64	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.12	J/mol×K	528.72	Joback Method
cpg	490.92	J/mol×K	558.32	Joback Method
cpg	507.98	J/mol×K	587.93	Joback Method
cpg	524.33	J/mol×K	617.53	Joback Method
cpg	539.98	J/mol×K	647.14	Joback Method
cpg	554.96	J/mol×K	676.74	Joback Method
cpg	569.28	J/mol×K	706.35	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	397.00	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65575e+01
Coeff. B	-5.18082e+03
Coeff. C	-9.00450e+01
Temperature range (K), min.	408.48
Temperature range (K), max.	550.73

Sources

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=C35216116&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

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