

5-Tetradecyne

Other names:	5-C14H26
Inchi:	InChI=1S/C14H26/c1-3-5-7-9-11-13-14-12-10-8-6-4-2/h3-9,11,13-14H2,1-2H3
InchiKey:	WHRIRYDVFUEMDX-UHFFFAOYSA-N
Formula:	C14H26
SMILES:	CCCCC#CCCCCCCCC
Mol. weight [g/mol]:	194.36
CAS:	60212-34-2

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	9.10 ± 0.03	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
ripol	1404.00		NIST Webbook
ripol	1404.00		NIST Webbook
ripol	1405.00		NIST Webbook
ripol	1421.00		NIST Webbook
ripol	1568.60		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1546.90		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1568.60		NIST Webbook
tb	528.72	K	Joback Method
tc	706.35	K	Joback Method
tf	353.64	K	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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51779e+01
Coeff. B	-4.71174e+03
Coeff. C	-7.77740e+01
Temperature range (K), min.	394.21
Temperature range (K), max.	555.33

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C60212342&Units=SI>

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
hvac:	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

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