

4-Tetradecyne

Other names:	4-C ₁₄ H ₂₆
Inchi:	InChI=1S/C14H26/c1-3-5-7-9-11-13-14-12-10-8-6-4-2/h3-7,9,11-14H2,1-2H3
InchiKey:	QWZXVDGVISCHQH-UHFFFAOYSA-N
Formula:	C ₁₄ H ₂₆
SMILES:	CCCC#CCCCCCCCCCC
Mol. weight [g/mol]:	194.36
CAS:	60212-33-1

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	9.11 ± 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	1407.00		NIST Webbook
ripol	1406.00		NIST Webbook
ripol	1407.00		NIST Webbook
ripol	1427.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1557.80		NIST Webbook
ripol	1553.60		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1585.00		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1576.30		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1557.80		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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60212331&Units=SI
Crippen Method:	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

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
mccvol:	McGowan's characteristic volume
pc:	Critical 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

Latest version available from:

<https://www.cheméo.com/cid/27-274-8/4-Tetradecyne.pdf>

Generated by Cheméo on 2024-04-25 08:40:20.605834846 +0000 UTC m=+16323669.526412161.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.