3-Tetradecyne

Other names: 3-C14H26
Inchi: InChI=1S/C14H26/c1-3-5-7-9-11-13-14-12-10-8-6-4-2/h3-5,7,9-14H2,1-2H3
InchiKey: DWWMJIDVLGUCDE-UHFFFAOYSA-N
Formula: C14H26
SMILES: CCC#CCCCCCCCCCC
Mol. weight [g/mol]: 194.36
CAS: 60212-32-0

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
log10ws	-5.48		Crippen Method
logp	4.931		Crippen Method
mcvol	199.520	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
ripol	1576.40		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1596.00		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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58335e+01
Coeff. B	-4.88986e+03
Coeff. C	-8.79760e+01
Temperature range (K), min.	402.52
Temperature range (K), max.	552.70

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60212320&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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
pvap: Vapor pressure

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