

7-Tetradecanone

Inchi:	InChI=1S/C14H28O/c1-3-5-7-9-11-13-14(15)12-10-8-6-4-2/h3-13H2,1-2H3
InchiKey:	ZEKPOTWCBTUBEB-UHFFFAOYSA-N
Formula:	C14H28O
SMILES:	CCCCCCCC(=O)CCCCC
Mol. weight [g/mol]:	212.37
CAS:	---

Physical Properties

Property code	Value	Unit	Source
gf	-61.92	kJ/mol	Joback Method
hf	-444.87	kJ/mol	Joback Method
hfus	33.61	kJ/mol	Joback Method
hvap	53.50	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.886		Crippen Method
mvol	209.690	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	1554.00		NIST Webbook
tb	573.59	K	Joback Method
tc	741.67	K	Joback Method
tf	297.47	K	Joback Method
vc	0.826	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.57	J/molxK	573.59	Joback Method
cpg	554.73	J/molxK	601.60	Joback Method
cpg	571.17	J/molxK	629.62	Joback Method
cpg	586.91	J/molxK	657.63	Joback Method
cpg	601.98	J/molxK	685.64	Joback Method
cpg	616.40	J/molxK	713.66	Joback Method
cpg	630.18	J/molxK	741.67	Joback Method
dvisc	0.0040142	Paxs	297.47	Joback Method

dvisc	0.0017253	Paxs	343.49	Joback Method
dvisc	0.0009053	Paxs	389.51	Joback Method
dvisc	0.0005444	Paxs	435.53	Joback Method
dvisc	0.0003608	Paxs	481.55	Joback Method
dvisc	0.0002569	Paxs	527.57	Joback Method
dvisc	0.0001932	Paxs	573.59	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52122e+01
Coeff. B	-4.83443e+03
Coeff. C	-9.40360e+01
Temperature range (K), min.	417.96
Temperature range (K), max.	582.33

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R319152&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/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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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