2-Hexene, 2,5-dimethyl-

Other names: 2,5-Dimethyl-2-hexene
2,5-Dimethylhex-2-ene
Inchi: InChI=1S/C8H16/c1-7(2)5-6-8(3)4/h5,8H,6H2,1-4H3
InchiKey: VFZIUYUUQFYZBR-UHFFFAOYSA-N
Formula: C8H16
SMILES: CC(C)=CCC(C)C
Mol. weight [g/mol]: 112.21
CAS: 3404-78-2

Physical Properties

Property code	Value	Unit	Source
gf	85.71	kJ/mol	Joback Method
hf	-106.30	kJ/mol	Joback Method
hfus	11.84	kJ/mol	Joback Method
hvap	38.90	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	749.80		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	750.50		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	751.00		NIST Webbook

rinpol	750.00		NIST Webbook
rinpol	749.50		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	762.00		NIST Webbook
tb	385.65 ± 4.00	K	NIST Webbook
tc	565.46	K	Joback Method
tf	145.88	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.93	J/mol×K	386.04	Joback Method
cpg	231.45	J/mol×K	415.94	Joback Method
cpg	244.37	J/mol×K	445.85	Joback Method
cpg	256.71	J/mol×K	475.75	Joback Method
cpg	268.50	J/mol×K	505.65	Joback Method
cpg	279.75	J/mol×K	535.55	Joback Method
cpg	290.49	J/mol×K	565.46	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38144e+01
Coeff. B	-2.97787e+03
Coeff. C	-6.18290e+01
Temperature range (K), min.	281.98
Temperature range (K), max.	412.05

Sources

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol298.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3404782&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume