Heptane, 2,2,6,6-tetramethyl-4-methylene-

Other names: 2-(2,2-dimethylpropyl)-4,4-dimethylpent-1-ene
4,4-Dimethyl-2-neopentyl-1-pentene
Inchi: InChI=1S/C12H24/c1-10(8-11(2,3)4)9-12(5,6)7/h1,8-9H2,2-7H3
InchiKey: TUFZRYOCZCLYJO-UHFFFAOYSA-N
Formula: C12H24
SMILES: C=C(CC(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]: 168.32
CAS: 141-70-8

Physical Properties

Property code	Value	Unit	Source
gf	135.13	kJ/mol	Joback Method
hf	-192.87	kJ/mol	Joback Method
hfus	9.42	kJ/mol	Joback Method
hvap	39.12	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.415		Crippen Method
mcvol	175.640	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
tb	464.06	K	Joback Method
tc	651.75	K	Joback Method
tf	248.00 ± 3.00	K	NIST Webbook
tf	249.60 ± 1.00	K	NIST Webbook
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.19	J/mol×K	464.06	Joback Method
cpg	412.64	J/mol×K	495.34	Joback Method
cpg	430.98	J/mol×K	526.62	Joback Method
cpg	448.29	J/mol×K	557.90	Joback Method
cpg	464.61	J/mol×K	589.18	Joback Method
cpg	479.99	J/mol×K	620.47	Joback Method

cpg	494.50	J/mol×K	651.75	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62756e+01
Coeff. B	-4.70208e+03
Coeff. C	-7.70880e+01
Temperature range (K), min.	371.19
Temperature range (K), max.	505.95

Sources

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=C141708&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume