3-Heptene, 2,2,4,6,6-pentamethyl-

Other names:	2,2,4,6,6-Pentamethyl-3-heptene
	2,2,4,6,6-Pentamethyl-3-heptene,c&t
	2,2,4,6,6-Pentamethylheptene-3
	2,2,4,6,6-pentamethylhept-3-ene
Inchi:	InChI=1S/C12H24/c1-10(8-11(2,3)4)9-12(5,6)7/h8H,9H2,1-7H3/b10-8+
InchiKey:	NBUMCEJRJRRLCA-CSKARUKUSA-N
Formula:	C12H24
SMILES:	CC(=CC(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]:	168.32
CAS:	123-48-8

Physical Properties

Property code	Value	Unit	Source
gf	127.51	kJ/mol	Joback Method
hf	-201.08	kJ/mol	Joback Method
hfus	10.90	kJ/mol	Joback Method
hvap	39.75	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.415		Crippen Method
mcvol	175.640	ml/mol	McGowan Method
pc	1932.13	kPa	Joback Method
tb	453.70 ± 2.00	K	NIST Webbook
tc	664.19	K	Joback Method
tf	210.80	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.23	J/mol×K	471.54	Joback Method
cpg	414.96	J/mol×K	503.65	Joback Method
cpg	433.53	J/mol×K	535.76	Joback Method
cpg	450.98	J/mol×K	567.87	Joback Method
cpg	467.39	J/mol×K	599.98	Joback Method

cpg	482.83	J/mol×K	632.09	Joback Method
cpg	497.35	J/mol×K	664.19	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50658e+01
Coeff. B	-4.03714e+03
Coeff. C	-6.72790e+01
Temperature range (K), min.	340.46
Temperature range (K), max.	481.16

Sources

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=C123488&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

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