3-Heptene, 2,2,3,5,5,6,6-heptamethyl-

Other names: 2,2,3,5,5,6,6-Heptamethyl-3-heptene
Inchi: InChI=1S/C14H28/c1-11(12(2,3)4)10-14(8,9)13(5,6)7/h10H,1-9H3/b11-10+
InchiKey: RVZGQICOUDJTHV-ZHACJKMWSA-N
Formula: C14H28
SMILES: CC(=CC(C)(C)C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 196.37
CAS: 54845-26-0

Physical Properties

Property code	Value	Unit	Source
gf	147.19	kJ/mol	Joback Method
hf	-251.11	kJ/mol	Joback Method
hfus	8.67	kJ/mol	Joback Method
hvap	42.91	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	5.051		Crippen Method
mcvol	203.820	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
tb	514.07	K	Joback Method
tc	713.84	K	Joback Method
tf	235.76	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.03	J/mol×K	514.07	Joback Method
cpg	518.17	J/mol×K	547.36	Joback Method
cpg	538.87	J/mol×K	580.66	Joback Method
cpg	558.23	J/mol×K	613.95	Joback Method
cpg	576.33	J/mol×K	647.25	Joback Method
cpg	593.27	J/mol×K	680.54	Joback Method
cpg	609.15	J/mol×K	713.84	Joback Method
hvapt	51.20	kJ/mol	329.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.21471e+01
Coeff. B	-3.32578e+03
Coeff. C	-7.46990e+01
Temperature range (K), min.	355.13
Temperature range (K), max.	561.24

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=C54845260&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
hvapt:	Enthalpy of vaporization at a given temperature
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