2,3,4-Trimethylpent-1-ene

Other names: 1-Pentene, 2,3,4-trimethyl-
2,3,4-Trimethyl-1-pentene
Inchi: InChI=1S/C8H16/c1-6(2)8(5)7(3)4/h7-8H,1H2,2-5H3
InchiKey: FAWUHEYSSPPNSH-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=C(C)C(C)C(C)C
Mol. weight [g/mol]: 112.21
CAS: 565-76-4

Physical Properties

Property code	Value	Unit	Source
gf	90.89	kJ/mol	Joback Method
hf	-103.37	kJ/mol	Joback Method
hfus	6.84	kJ/mol	Joback Method
hvap	38.50	kJ/mol	NIST Webbook
log10ws	-2.54		Crippen Method
logp	2.855		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpol	724.50		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	724.10		NIST Webbook
rinpol	728.70		NIST Webbook
rinpol	726.50		NIST Webbook
tb	381.20 ± 1.50	K	NIST Webbook
tb	381.00 ± 2.00	K	NIST Webbook
tb	117.00 ± 3.00	K	NIST Webbook
tc	556.32	K	Joback Method
tf	134.20	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	217.46	J/mol×K	378.12	Joback Method
cpg	230.96	J/mol×K	407.82	Joback Method
cpg	243.91	J/mol×K	437.52	Joback Method
cpg	256.31	J/mol×K	467.22	Joback Method
cpg	268.18	J/mol×K	496.92	Joback Method
cpg	279.54	J/mol×K	526.62	Joback Method
cpg	290.40	J/mol×K	556.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37044e+01
Coeff. B	-2.89114e+03
Coeff. C	-6.29560e+01
Temperature range (K), min.	278.44
Temperature range (K), max.	407.43

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=C565764&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume