1-Pentene, 2,3,3-trimethyl-

Other names: 2,3,3-Trimethyl-1-pentene
2,3,3-Trimethylpent-1-ene
Inchi: InChI=1S/C8H16/c1-6-8(4,5)7(2)3/h2,6H2,1,3-5H3
InchiKey: TUSBCMPNIOJUBX-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=C(C)C(C)(C)CC
Mol. weight [g/mol]: 112.21
CAS: 560-23-6

Physical Properties

Property code	Value	Unit	Source
gf	98.61	kJ/mol	Joback Method
hf	-101.56	kJ/mol	Joback Method
hfus	6.47	kJ/mol	Joback Method
hvap	38.50	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	738.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	730.50		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	743.30		NIST Webbook
rinpol	743.30		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	730.30		NIST Webbook
rinpol	743.00		NIST Webbook
tb	381.46 ± 0.25	K	NIST Webbook
tb	381.40 ± 1.00	K	NIST Webbook
tb	381.55 ± 0.30	K	NIST Webbook
tb	391.65 ± 0.30	K	NIST Webbook
tc	557.27	K	Joback Method

tf	204.00 ± 3.00	K	NIST Webbook
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.61	J/mol×K	375.77	Joback Method
cpg	232.95	J/mol×K	406.02	Joback Method
cpg	246.58	J/mol×K	436.27	Joback Method
cpg	259.50	J/mol×K	466.52	Joback Method
cpg	271.77	J/mol×K	496.77	Joback Method
cpg	283.40	J/mol×K	527.02	Joback Method
cpg	294.42	J/mol×K	557.27	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36323e+01
Coeff. B	-2.87503e+03
Coeff. C	-6.25060e+01
Temperature range (K), min.	277.95
Temperature range (K), max.	408.03

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C560236&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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol327.mol

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