2-Pentene, 2,3,4-trimethyl-

Other names: (CH3)2CHC(CH3)=C(CH3)2
2,3,4-Trimethyl-2-pentene
2,3,4-Trimethylpent-2-ene
Inchi: InChI=1S/C8H16/c1-6(2)8(5)7(3)4/h6H,1-5H3
InchiKey: SZFRZEBLZFTODC-UHFFFAOYSA-N
Formula: C8H16
SMILES: CC(C)=C(C)C(C)C
Mol. weight [g/mol]: 112.21
CAS: 565-77-5

Physical Properties

Property code	Value	Unit	Source
gf	77.16	kJ/mol	Joback Method
hf	-116.09	kJ/mol	Joback Method
hfus	10.54	kJ/mol	Joback Method
hvap	39.30	kJ/mol	NIST Webbook
ie	8.16 ± 0.01	eV	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	779.50		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	779.50		NIST Webbook
rinpol	764.80		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	773.50		NIST Webbook
rinpol	774.80		NIST Webbook
rinpol	765.70		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	773.50		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	766.00		NIST Webbook

rinpol	765.50		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	767.00		NIST Webbook
tb	387.00 ± 6.00	K	NIST Webbook
tb	389.55 ± 0.50	K	NIST Webbook
tb	389.65 ± 0.30	K	NIST Webbook
tb	389.35 ± 0.40	K	NIST Webbook
tb	389.70	K	NIST Webbook
tc	568.97	K	Joback Method
tf	159.77 ± 0.10	K	NIST Webbook
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.91	J/mol×K	385.92	Joback Method
cpg	231.67	J/mol×K	416.43	Joback Method
cpg	244.80	J/mol×K	446.94	Joback Method
cpg	257.34	J/mol×K	477.45	Joback Method
cpg	269.30	J/mol×K	507.96	Joback Method
cpg	280.70	J/mol×K	538.47	Joback Method
cpg	291.57	J/mol×K	568.97	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37872e+01
Coeff. B	-3.03972e+03
Coeff. C	-5.81740e+01
Temperature range (K), min.	283.34
Temperature range (K), max.	416.81

Sources

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/mol335.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C565775&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
ie:	Ionization energy
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