Z-3,4,4-Trimethyl-2-pentene

Other names: (2Z)-3,4,4-Trimethyl-2-pentene
(Z)-3,4,4-Trimethylpent-2-ene
2-Pentene, 3,4,4-trimethyl-, cis
3,4,4-Trimethyl-2-pentene, cis
3,4,4-Trimethyl-cis-2-pentene
Inchi: InChI=1S/C8H16/c1-6-7(2)8(3,4)5/h6H,1-5H3/b7-6-
InchiKey: FZQMZRXKWHQJAG-SREVYHEPSA-N
Formula: C8H16
SMILES: CC=C(C)C(C)(C)C
Mol. weight [g/mol]: 112.21
CAS: 39761-64-3

Physical Properties

Property code	Value	Unit	Source
gf	90.99	kJ/mol	Joback Method
hf	-109.77	kJ/mol	Joback Method
hfus	7.95	kJ/mol	Joback Method
hvap	38.90	kJ/mol	NIST Webbook
hvap	38.90	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	761.00		NIST Webbook
rinpol	766.20		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	758.40		NIST Webbook
rinpol	766.20		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	749.00		NIST Webbook
tb	385.45 ± 0.40	K	NIST Webbook
tc	570.42	K	Joback Method
tf	163.30	K	Joback Method

vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.11	J/mol×K	383.25	Joback Method
cpg	233.89	J/mol×K	414.44	Joback Method
cpg	247.86	J/mol×K	445.64	Joback Method
cpg	261.06	J/mol×K	476.83	Joback Method
cpg	273.52	J/mol×K	508.03	Joback Method
cpg	285.30	J/mol×K	539.22	Joback Method
cpg	296.41	J/mol×K	570.42	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34432e+01
Coeff. B	-2.79748e+03
Coeff. C	-6.84500e+01
Temperature range (K), min.	281.10
Temperature range (K), max.	412.47

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=C39761643&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
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