

trans-2,3-Dimethyl-2-pentene

Inchi:	InChI=1S/C7H14/c1-5-7(4)6(2)3/h5H2,1-4H3
InchiKey:	WFHALSLYRWWUGH-UHFFFAOYSA-N
Formula:	C7H14
SMILES:	CCC(C)=C(C)C
Mol. weight [g/mol]:	98.19

Physical Properties

Property code	Value	Unit	Source
gf	71.18	kJ/mol	Joback Method
hf	-90.17	kJ/mol	Joback Method
hfus	11.47	kJ/mol	Joback Method
hvap	31.29	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.753		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	712.00		NIST Webbook
tb	363.48	K	Joback Method
tc	542.91	K	Joback Method
tf	135.65	K	Joback Method
vc	0.409	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.35	J/mol×K	363.48	Joback Method
cpg	192.44	J/mol×K	393.38	Joback Method
cpg	204.00	J/mol×K	423.29	Joback Method
cpg	215.05	J/mol×K	453.19	Joback Method
cpg	225.59	J/mol×K	483.10	Joback Method
cpg	235.66	J/mol×K	513.00	Joback Method
cpg	245.27	J/mol×K	542.91	Joback Method

Sources

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=R643277&Units=SI
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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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