

cis-1,1,1-Trimethyl-2-butene

Inchi:	InChI=1S/C7H14/c1-5-6-7(2,3)4/h5-6H,1-4H3/b6-5-
InchiKey:	BIDIHFPLDRSAMB-WAYWQWQTSA-N
Formula:	C7H14
SMILES:	CC=CC(C)(C)C
Mol. weight [g/mol]:	98.19

Physical Properties

Property code	Value	Unit	Source
gf	91.12	kJ/mol	Joback Method
hf	-79.34	kJ/mol	Joback Method
hfus	6.67	kJ/mol	Joback Method
hvap	29.84	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	638.00		NIST Webbook
rinpol	638.00		NIST Webbook
tb	360.49	K	Joback Method
tc	544.64	K	Joback Method
tf	165.99	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.91	J/mol×K	360.49	Joback Method
cpg	194.27	J/mol×K	391.18	Joback Method
cpg	206.90	J/mol×K	421.87	Joback Method
cpg	218.84	J/mol×K	452.57	Joback Method
cpg	230.11	J/mol×K	483.26	Joback Method
cpg	240.74	J/mol×K	513.95	Joback Method
cpg	250.78	J/mol×K	544.64	Joback Method
dvisc	0.0108776	Pa×s	165.99	Joback Method

dvisc	0.0033838	Pa×s	198.41	Joback Method
dvisc	0.0014612	Pa×s	230.82	Joback Method
dvisc	0.0007760	Pa×s	263.24	Joback Method
dvisc	0.0004734	Pa×s	295.66	Joback Method
dvisc	0.0003185	Pa×s	328.07	Joback Method
dvisc	0.0002301	Pa×s	360.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R634045&Units=SI
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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log_{10ws}:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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