

Tricyclo[2.2.1.0(2,6)]heptane, 1,7,7-trimethyl-

Other names:	Tricyclene 1,7,7-Trimethyltricyclo[2.2.1.0,2,6]heptane Cyclene NSC 86978 1,7,7-Trimethyl-tricyclo[2.2.1.0*2,6*]heptane «alpha»-Tricyclene Tricyclo[2.2.1.02,6]heptane, 1,7,7-trimethyl- 1,7,7-trimethyltricyclo[2.2.1.02,6]heptane
Inchi:	InChI=1S/C10H16/c1-9(2)6-4-7-8(5-6)10(7,9)3/h6-8H,4-5H2,1-3H3
InchiKey:	RRBYUSWBLVXTQN-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	CC1(C)C2CC3C(C2)C31C
Mol. weight [g/mol]:	136.23
CAS:	508-32-7

Physical Properties

Property code	Value	Unit	Source
chs	-6146.70	kJ/mol	NIST Webbook
gf	213.37	kJ/mol	Joback Method
hf	-29.21	kJ/mol	Joback Method
hfus	9.81	kJ/mol	Joback Method
hvap	34.33	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.688		Crippen Method
mcvol	119.180	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
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ripol	1003.00		NIST Webbook
tb	426.70	K	NIST Webbook
tc	637.57	K	Joback Method
tf	302.64	K	Joback Method
vc	0.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.10	J/mol×K	431.02	Joback Method
cpg	294.56	J/mol×K	465.45	Joback Method
cpg	312.07	J/mol×K	499.87	Joback Method
cpg	327.87	J/mol×K	534.30	Joback Method
cpg	342.20	J/mol×K	568.72	Joback Method
cpg	355.32	J/mol×K	603.15	Joback Method
cpg	367.47	J/mol×K	637.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C508327&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

chs:	Standard solid enthalpy of combustion
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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
ri_{pol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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