

Tricyclo[2.2.1.0(2,6)]heptane, 1,3,3-trimethyl-

Other names:	Cyclofenchene Tricyclo[2.2.1.02,6]heptane, 1,3,3-trimethyl- 1,3,3-trimethyltricyclo[2.2.1.02,6]heptane
Inchi:	InChI=1S/C10H16/c1-9(2)6-4-7-8(9)10(7,3)5-6/h6-8H,4-5H2,1-3H3
InchiKey:	NZXWDTCLMXDSHY-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	CC1(C)C2CC3C1C3(C)C2
Mol. weight [g/mol]:	136.23
CAS:	488-97-1

Physical Properties

Property code	Value	Unit	Source
chl	-6155.10	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
rinpol	890.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	882.10		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	927.00		NIST Webbook
ripol	946.00		NIST Webbook
tb	431.02	K	Joback Method
tc	637.57	K	Joback Method
tf	302.64	K	Joback Method
vc	0.476	m3/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

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=C488971&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid 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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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