

Bicyclo[2.2.1]heptane, 2,2,3-trimethyl-

Other names:	Isocamphane
	Dihydrocamphene
Inchi:	InChI=1S/C10H18/c1-7-8-4-5-9(6-8)10(7,2)3/h7-9H,4-6H2,1-3H3
InchiKey:	XETQTCAMTVHYPO-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	CC1C2CCC(C2)C1(C)C
Mol. weight [g/mol]:	138.25
CAS:	473-19-8

Physical Properties

Property code	Value	Unit	Source
gf	121.81	kJ/mol	Joback Method
hf	-135.73	kJ/mol	Joback Method
hfus	11.67	kJ/mol	Joback Method
hvap	36.08	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	3.079		Crippen Method
mcvol	130.040	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1060.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1052.00		NIST Webbook
ripol	1134.00		NIST Webbook
tb	436.85	K	Joback Method
tc	642.10	K	Joback Method
tf	360.00 ± 6.00	K	NIST Webbook
tf	427.00 ± 2.50	K	NIST Webbook
tf	336.70 ± 0.50	K	NIST Webbook
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	287.02	J/mol×K	436.85	Joback Method
cpg	307.28	J/mol×K	471.06	Joback Method
cpg	326.14	J/mol×K	505.27	Joback Method
cpg	343.70	J/mol×K	539.47	Joback Method
cpg	360.10	J/mol×K	573.68	Joback Method
cpg	375.46	J/mol×K	607.89	Joback Method
cpg	389.91	J/mol×K	642.10	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=C473198&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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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