

Tricyclo[3.2.1.0^{2,4}]octane,(1 «alpha»,2«alpha»,4«alpha»)

Inchi:	InChI=1S/C8H12/c1-2-6-3-5(1)7-4-8(6)7/h5-8H,1-4H2/t5-,6-,7-,8+/m1/s1
InchiKey:	PSZPCAFRANQPLS-XUTV FYLZSA-N
Formula:	C8H12
SMILES:	C1CC2CC1C1CC21
Mol. weight [g/mol]:	108.18
CAS:	22389-16-8

Physical Properties

Property code	Value	Unit	Source
gf	203.12	kJ/mol	Joback Method
hf	-4.23	kJ/mol	Joback Method
hfus	14.05	kJ/mol	Joback Method
hvap	32.66	kJ/mol	Joback Method
ie	9.40	eV	NIST Webbook
ie	8.80 ± 0.10	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	2.052		Crippen Method
mcvol	91.000	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	393.72	K	Joback Method
tc	594.92	K	Joback Method
tf	233.02	K	Joback Method
vc	0.361	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.89	J/mol×K	393.72	Joback Method
cpg	262.25	J/mol×K	561.38	Joback Method
cpg	249.40	J/mol×K	527.85	Joback Method
cpg	235.52	J/mol×K	494.32	Joback Method
cpg	220.54	J/mol×K	460.79	Joback Method
cpg	204.36	J/mol×K	427.25	Joback Method
cpg	274.16	J/mol×K	594.92	Joback Method

dvisc	0.0008202	Paxs	393.72	Joback Method
dvisc	0.0006884	Paxs	366.94	Joback Method
dvisc	0.0005621	Paxs	340.15	Joback Method
dvisc	0.0004433	Paxs	313.37	Joback Method
dvisc	0.0003344	Paxs	286.59	Joback Method
dvisc	0.0002381	Paxs	259.80	Joback Method
dvisc	0.0001567	Paxs	233.02	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=C22389168&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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