

Tetracyclo[3.3.1.0(2,8).0(4,6)]nonane

Other names:	Triasterane
Inchi:	InChI=1S/C9H12/c1-4-6-2-7-5(1)9(7)3-8(4)6/h4-9H,1-3H2
InchiKey:	YTFCTXSQPWYFH-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	C1C2C3CC4C1C4CC23
Mol. weight [g/mol]:	120.19
CAS:	3105-29-1

Physical Properties

Property code	Value	Unit	Source
gf	288.78	kJ/mol	Joback Method
hf	39.91	kJ/mol	Joback Method
hfus	20.05	kJ/mol	Joback Method
hvap	34.15	kJ/mol	Joback Method
ie	8.20	eV	NIST Webbook
ie	8.67	eV	NIST Webbook
log10ws	-1.72		Crippen Method
logp	1.908		Crippen Method
mcvol	94.230	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
tb	410.13	K	Joback Method
tc	609.46	K	Joback Method
tf	265.03	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.86	J/mol×K	410.13	Joback Method
cpg	293.88	J/mol×K	576.24	Joback Method
cpg	280.79	J/mol×K	543.02	Joback Method
cpg	266.56	J/mol×K	509.80	Joback Method
cpg	251.07	J/mol×K	476.57	Joback Method
cpg	234.21	J/mol×K	443.35	Joback Method

cpg	305.94	J/mol×K	609.46	Joback Method
dvisc	0.0018785	Pa×s	410.13	Joback Method
dvisc	0.0013753	Pa×s	385.95	Joback Method
dvisc	0.0009657	Pa×s	361.76	Joback Method
dvisc	0.0006447	Pa×s	337.58	Joback Method
dvisc	0.0004043	Pa×s	313.40	Joback Method
dvisc	0.0002345	Pa×s	289.21	Joback Method
dvisc	0.0001232	Pa×s	265.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3105291&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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