

(3S,3aS,6R,8aS)-3,8,8-Trimethyl-7-methyloctane

Other names:	Prezizaene Preziza-7(15)-ene
Inchi:	InChI=1S/C15H24/c1-10-5-6-13-14(3,4)11(2)12-7-8-15(10,13)9-12/h10,12-13H,2,5-9H2,1
InchiKey:	RFSYBMDOYOBTCL-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	C=C1C2CCC3(C2)C(C)CCC3C1(C)C
Mol. weight [g/mol]:	204.35
CAS:	31145-21-8

Physical Properties

Property code	Value	Unit	Source
gf	260.15	kJ/mol	Joback Method
hf	-72.81	kJ/mol	Joback Method
hfus	13.20	kJ/mol	Joback Method
hvap	46.31	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinp	1444.00		NIST Webbook
rinp	1444.00		NIST Webbook
tb	561.66	K	Joback Method
tc	785.91	K	Joback Method
tf	358.59	K	Joback Method
vc	0.709	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.94	J/molxK	561.66	Joback Method
cpg	525.20	J/molxK	599.03	Joback Method
cpg	546.85	J/molxK	636.41	Joback Method
cpg	567.18	J/molxK	673.78	Joback Method
cpg	586.48	J/molxK	711.16	Joback Method

cpg	605.02	J/mol×K	748.53	Joback Method
cpg	623.10	J/mol×K	785.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C31145218&Units=SI

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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