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

Other names:	Khusimene
	Zizaene
	Khusene
	Ziza-6(13)-ene
Inchi:	InChI=1S/C15H24/c1-10-5-6-13-11(2)14(3,4)12-7-8-15(10,13)9-12/h10,12-13H,2,5-9H2,1
InchiKey:	VBZRHXLPRWBPEH-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	C=C1C2CCC(C)C23CCC(C3)C1(C)C
Mol. weight [g/mol]:	204.35
CAS:	18444-94-5

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
rinpol	1453.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1457.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1597.00		NIST Webbook

tb	561.66	K	Joback Method
tc	785.91	K	Joback Method
tf	358.59	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18444945&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

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
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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