

Khusimene

Inchi:	InChI=1S/C15H24/c1-10-5-7-12-9-15(14(12,3)4)11(2)6-8-13(10)15/h11-13H,1,5-9H2,2-4
InchiKey:	HOMAFFTYQJEIDP-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	C=C1CCC2CC3(C(C)CCC13)C2(C)C
Mol. weight [g/mol]:	204.35

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	1455.00		NIST Webbook
rinpol	1455.00		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/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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R625591&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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