

Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methyl-4«beta»,7«beta»,8«alpha»)-[1R-(1«alpha»,7«beta»,8«alpha»)]-Valencene

Other names:	4«beta»,7«beta»,8«alpha»-Fremochila-1(10),11-diene (+)-Valencene Valencen Valencene 4«alpha»,10«alpha»-Dimethyl-6«beta»-isopropyl-«delta»1,9-octalin Valencene 85 [1R-(1«alpha»,7«beta»,8«alpha»)]-1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methyl-4«beta»,7«beta»,8«alpha»)-Fremochila-1(10),11-diene
Inchi:	InChI=1S/C15H24/c1-11(2)13-8-9-14-7-5-6-12(3)15(14,4)10-13/h7,12-13H,1,5-6,8-10H2,11H
InchiKey:	QEBNYNLSCGVZOH-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	C=C(C)C1CCC2=CCCC(C)C2(C)C1
Mol. weight [g/mol]:	204.35
CAS:	4630-07-3

Physical Properties

Property code	Value	Unit	Source
gf	234.94	kJ/mol	Joback Method
hf	-75.12	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
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tb	569.43	K	Joback Method
tc	794.31	K	Joback Method
tf	297.83	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.65	J/mol×K	569.43	Joback Method
cpg	523.17	J/mol×K	606.91	Joback Method
cpg	545.19	J/mol×K	644.39	Joback Method
cpg	565.88	J/mol×K	681.87	Joback Method
cpg	585.40	J/mol×K	719.35	Joback Method
cpg	603.90	J/mol×K	756.83	Joback Method
cpg	621.57	J/mol×K	794.31	Joback Method

Sources

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=C4630073&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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