

Tetrahydrothujopsene-a

Inchi:

InChI=1S/C15H26/c1-11-6-9-14(4)8-5-7-13(2,3)15(14)10-12(11)15/h11-12H,5-10H2,1-4H

InchiKey:

OECAXGZVYRHQKP-ZJPTYJIISA-N

Formula:

C15H26

SMILES:

CC1CCC2(C)CCCC(C)(C)C23CC13

Mol. weight [g/mol]:

206.37

Physical Properties

Property code	Value	Unit	Source
gf	201.58	kJ/mol	Joback Method
hf	-141.81	kJ/mol	Joback Method
hfus	8.06	kJ/mol	Joback Method
hvap	45.00	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.639		Crippen Method
mcvol	189.630	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1496.00		NIST Webbook
rinpol	1496.00		NIST Webbook
ripol	1668.00		NIST Webbook
tb	562.74	K	Joback Method
tc	794.27	K	Joback Method
tf	368.81	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.13	J/mol×K	562.74	Joback Method
cpg	545.62	J/mol×K	601.33	Joback Method
cpg	568.31	J/mol×K	639.92	Joback Method
cpg	589.63	J/mol×K	678.51	Joback Method
cpg	610.00	J/mol×K	717.09	Joback Method
cpg	629.86	J/mol×K	755.68	Joback Method
cpg	649.64	J/mol×K	794.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R306597&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
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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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