

Myltayl-4(12)-ene

Other names:	(-)-Myltayl-4(12)-ene
Inchi:	InChI=1S/C15H24/c1-11-10-15-9-6-12(11)14(15,4)8-5-7-13(15,2)3/h12H,1,5-10H2,2-4H3
InchiKey:	PNEUWJHYPHTVCH-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	C=C1CC23CCC1C2(C)CCCC3(C)C
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	262.37	kJ/mol	Joback Method
hf	-37.23	kJ/mol	Joback Method
hfus	5.83	kJ/mol	Joback Method
hvap	45.46	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1455.00		NIST Webbook
rinpol	1455.00		NIST Webbook
tb	566.57	K	Joback Method
tc	800.20	K	Joback Method
tf	386.73	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.14	J/molxK	566.57	Joback Method
cpg	522.76	J/molxK	605.51	Joback Method
cpg	543.69	J/molxK	644.45	Joback Method
cpg	563.39	J/molxK	683.38	Joback Method
cpg	582.28	J/molxK	722.32	Joback Method
cpg	600.82	J/molxK	761.26	Joback Method
cpg	619.44	J/molxK	800.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R430596&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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