

2,6,10,14-Tetramethyl-9-(3-methyl-pent-4-enyliden)

Inchi:	InChI=1S/C25H44/c1-9-22(6)16-18-25(24(8)15-11-13-21(4)5)19-17-23(7)14-10-12-20(2)
InchiKey:	NGTHMXZCVWHQKA-VAHBTUPDSA-N
Formula:	C25H44
SMILES:	C=CC(C)CC=C(CC=C(C)CCC=C(C)C)C(C)CCCC(C)C
Mol. weight [g/mol]:	344.62

Physical Properties

Property code	Value	Unit	Source
gf	455.15	kJ/mol	Joback Method
hf	-127.45	kJ/mol	Joback Method
hfus	45.33	kJ/mol	Joback Method
hvap	69.52	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	8.670		Crippen Method
mcvol	345.910	ml/mol	McGowan Method
pc	874.80	kPa	Joback Method
rinpol	2130.00		NIST Webbook
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	778.88	K	Joback Method
tc	966.44	K	Joback Method
tf	267.63	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.63	J/molxK	778.88	Joback Method
cpg	1075.61	J/molxK	810.14	Joback Method
cpg	1096.54	J/molxK	841.40	Joback Method
cpg	1116.50	J/molxK	872.66	Joback Method
cpg	1135.60	J/molxK	903.92	Joback Method
cpg	1153.89	J/molxK	935.18	Joback Method
cpg	1171.47	J/molxK	966.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R274554&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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