

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

Inchi: InChI=1S/C25H42/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: VDOFLWFFQCRKTK-BRYXKCCLSA-N
Formula: C25H42
SMILES: C=CC(C)CC=C(CC=C(C)CCC=C(C)C)C(C)CCC=C(C)C
Mol. weight [g/mol]: 342.60

Physical Properties

Property code	Value	Unit	Source
gf	529.26	kJ/mol	Joback Method
hf	-14.74	kJ/mol	Joback Method
hfus	47.75	kJ/mol	Joback Method
hvap	69.95	kJ/mol	Joback Method
log10ws	-9.07		Crippen Method
logp	8.590		Crippen Method
mcvol	341.610	ml/mol	McGowan Method
pc	900.72	kPa	Joback Method
rinpol	2112.00		NIST Webbook
rinpol	2112.00		NIST Webbook
rinpol	2126.00		NIST Webbook
tb	783.36	K	Joback Method
tc	974.84	K	Joback Method
tf	263.59	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.64	J/molxK	783.36	Joback Method
cpg	1050.17	J/molxK	815.27	Joback Method
cpg	1070.69	J/molxK	847.19	Joback Method
cpg	1090.32	J/molxK	879.10	Joback Method
cpg	1109.15	J/molxK	911.01	Joback Method
cpg	1127.28	J/molxK	942.92	Joback Method
cpg	1144.80	J/molxK	974.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R274529&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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