

2,6,10,14-Tetramethyl-7-(3-methyl-pent-4-enyl)-pentane

Inchi:

lnchl=1S/C25H46/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:

XZZXYRIDRYGHIR-BXPHKCKFSA-N

Formula:

C25H46

SMILES:

C=CC(C)CCC(CC=C(C)CCCC(C)C)C(C)=CCCC(C)C

Mol. weight [g/mol]:

346.63

Physical Properties

Property code	Value	Unit	Source
gf	381.04	kJ/mol	Joback Method
hf	-240.16	kJ/mol	Joback Method
hfus	42.92	kJ/mol	Joback Method
hvap	69.10	kJ/mol	Joback Method
log10ws	-8.88		Crippen Method
logp	8.750		Crippen Method
mcvol	350.210	ml/mol	McGowan Method
pc	849.99	kPa	Joback Method
rinpol	2103.00		NIST Webbook
rinpol	2103.00		NIST Webbook
rinpol	2106.00		NIST Webbook
rinpol	2103.00		NIST Webbook
tb	774.40	K	Joback Method
tc	958.36	K	Joback Method
tf	271.67	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.38	J/mol×K	774.40	Joback Method
cpg	1100.83	J/mol×K	805.06	Joback Method
cpg	1122.19	J/mol×K	835.72	Joback Method
cpg	1142.53	J/mol×K	866.38	Joback Method
cpg	1161.93	J/mol×K	897.04	Joback Method
cpg	1180.45	J/mol×K	927.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R500744&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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