

2,6,14-Trimethyl-10-methylene-9-(3-methyl-pent-4-

Inchi:

LnChI=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:

QNCQOYEQQDOUCMW-HAVVHWLPSA-N

Formula:

C25H44

SMILES:

C=CC(C)CCC(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	462.77	kJ/mol	Joback Method
hf	-119.24	kJ/mol	Joback Method
hfus	43.85	kJ/mol	Joback Method
hvap	68.90	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	8.670		Crippen Method
mcvol	345.910	ml/mol	McGowan Method
pc	869.65	kPa	Joback Method
rinpol	2140.00		NIST Webbook
rinpol	2145.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2145.50		NIST Webbook
rinpol	2140.00		NIST Webbook
ripol	2238.00		NIST Webbook
ripol	2232.00		NIST Webbook
ripol	2232.00		NIST Webbook
tb	771.40	K	Joback Method
tc	956.38	K	Joback Method
tf	270.95	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1051.00	J/mol×K	771.40	Joback Method
cpg	1072.94	J/mol×K	802.23	Joback Method

cpg	1093.82	J/mol×K	833.06	Joback Method
cpg	1113.72	J/mol×K	863.89	Joback Method
cpg	1132.71	J/mol×K	894.72	Joback Method
cpg	1150.87	J/mol×K	925.55	Joback Method
cpg	1168.26	J/mol×K	956.38	Joback Method

Sources

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=R278383&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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