

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

Inchi:	InChI=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:	BSXYLMVBPPIDSG-HAVVHWLPSA-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	388.66	kJ/mol	Joback Method
hf	-231.95	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	68.47	kJ/mol	Joback Method
log10ws	-8.88		Crippen Method
logp	8.750		Crippen Method
mcvol	350.210	ml/mol	McGowan Method
pc	845.05	kPa	Joback Method
rinpol	2106.00		NIST Webbook
rinpol	2106.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	766.92	K	Joback Method
tc	948.41	K	Joback Method
tf	274.99	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.51	J/molxK	766.92	Joback Method
cpg	1097.95	J/molxK	797.17	Joback Method
cpg	1119.28	J/molxK	827.42	Joback Method
cpg	1139.59	J/molxK	857.67	Joback Method
cpg	1158.92	J/molxK	887.92	Joback Method
cpg	1177.35	J/molxK	918.17	Joback Method
cpg	1194.92	J/molxK	948.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R500779&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

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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