

1-Methyl-4-(1-methylethenyl)-3-[1-methyl-1-(4-methyl-1-cyclohexenyl)-3-[1,5-Dimethyl-1-(4-methyl-pentyl)--hept-6-enyl]-4-isopropenyl-1-methyl-cyclohexene

Other names:
InChI: InChI=1S/C25H44/c1-9-21(6)13-11-17-25(8,16-10-12-19(2)3)24-18-22(7)14-15-23(24)20
InchiKey: BOZVIOBNRKAICT-UHFFFAOYSA-N
Formula: C25H44
SMILES: C=CC(C)CCCC(C)(CCCC(C)C)C1C=C(C)CCC1C(=C)C
Mol. weight [g/mol]: 344.62

Physical Properties

Property code	Value	Unit	Source
gf	361.78	kJ/mol	Joback Method
hf	-257.28	kJ/mol	Joback Method
hfus	35.91	kJ/mol	Joback Method
hvap	68.99	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	8.360		Crippen Method
mcvol	339.350	ml/mol	McGowan Method
pc	917.72	kPa	Joback Method
rinpol	2089.00		NIST Webbook
rinpol	2102.00		NIST Webbook
tb	779.55	K	Joback Method
tc	974.84	K	Joback Method
tf	342.87	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.37	J/mol×K	779.55	Joback Method
cpg	1099.11	J/mol×K	812.10	Joback Method
cpg	1121.48	J/mol×K	844.65	Joback Method
cpg	1142.57	J/mol×K	877.19	Joback Method
cpg	1162.43	J/mol×K	909.74	Joback Method
cpg	1181.15	J/mol×K	942.29	Joback Method
cpg	1198.79	J/mol×K	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=U370413&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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