

Cyclopentane, 1-ethyl-1-methyl-3-(1,5-dimethylhexyl)-2-(2,6,10-trimethylundecyl)isomer # 1

InChI: InChI=1S/C32H64/c1-10-12-17-26(5)18-14-19-27(6)20-15-22-29(8)31-30(23-24-32(31,9)
InChIKey: ZUAGKGLTGFTOFN-UHFFFAOYSA-N

Formula: C32H64

SMILES: CCCCC(C)CCCC(C)CCCC(C)C1C(C(C)CCCC(C)C)CCC1(C)CC

Mol. weight [g/mol]: 448.85

Physical Properties

Property code	Value	Unit	Source
gf	222.00	kJ/mol	Joback Method
hf	-695.17	kJ/mol	Joback Method
hfus	50.80	kJ/mol	Joback Method
hvap	83.37	kJ/mol	Joback Method
log10ws	-11.18		Crippen Method
logp	11.330		Crippen Method
mcvol	450.880	ml/mol	McGowan Method
pc	597.50	kPa	Joback Method
rinpol	2506.00		NIST Webbook
rinpol	2506.00		NIST Webbook
tb	935.54	K	Joback Method
tc	1145.96	K	Joback Method
tf	401.72	K	Joback Method
vc	1.734	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1622.16	J/molxK	935.54	Joback Method
cpg	1652.34	J/molxK	970.61	Joback Method
cpg	1681.55	J/molxK	1005.68	Joback Method
cpg	1709.95	J/molxK	1040.75	Joback Method
cpg	1737.71	J/molxK	1075.82	Joback Method
cpg	1765.01	J/molxK	1110.89	Joback Method
cpg	1792.01	J/molxK	1145.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R619031&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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