1,4,6-Trimethyl-1,2,3,3a,4,7,8,8a-octahydro-4,7-eth

Other names: Rotundene
Inchi: InChI=1S/C15H24/c1-10-4-5-14-13(10)8-12-6-7-15(14,3)9-11(12)2/h9-10,12-14H,4-8H2,
InchiKey: XAAMMPKFMNZIIC-UHFFFAOYSA-N
Formula: C15H24
SMILES: CC1=CC2(C)CCC1CC1C(C)CCC12
Mol. weight [g/mol]: 204.35
CAS: 65128-08-7

Physical Properties

Property code	Value	Unit	Source
gf	220.79	kJ/mol	Joback Method
hf	-132.14	kJ/mol	Joback Method
hfus	19.39	kJ/mol	Joback Method
hvap	48.42	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	1468.00		NIST Webbook
rinpol	1460.00		NIST Webbook
tb	570.67	K	Joback Method
tc	795.06	K	Joback Method
tf	330.77	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.52	J/mol×K	570.67	Joback Method
cpg	530.69	J/mol×K	608.07	Joback Method
cpg	553.27	J/mol×K	645.47	Joback Method
cpg	574.46	J/mol×K	682.86	Joback Method
cpg	594.42	J/mol×K	720.26	Joback Method
cpg	613.36	J/mol×K	757.66	Joback Method

cpg	631.47	J/mol×K	795.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65128087&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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