«gamma»-Cuprenene

Inchi: InChI=1S/C15H24/c1-12-6-8-13(9-7-12)15(4)11-5-10-14(15,2)3/h6,9H,5,7-8,10-11H2,1-4
InchiKey: MDJJOJZGNNCGHU-UHFFFAOYSA-N
Formula: C15H24
SMILES: CC1=CCC(C2(C)CCCC2(C)C)=CC1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	166.10	kJ/mol	Joback Method
hf	-115.03	kJ/mol	Joback Method
hfus	9.45	kJ/mol	Joback Method
hvap	49.28	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1537.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1523.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1707.00		NIST Webbook
tb	586.19	K	Joback Method
tc	822.53	K	Joback Method
tf	351.45	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	500.78	J/mol×K	586.19	Joback Method
cpg	523.43	J/mol×K	625.58	Joback Method
cpg	544.65	J/mol×K	664.97	Joback Method
cpg	564.73	J/mol×K	704.36	Joback Method
cpg	583.94	J/mol×K	743.75	Joback Method
cpg	602.58	J/mol×K	783.14	Joback Method
cpg	620.93	J/mol×K	822.53	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=R209644&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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