Cyclosativene

Inchi: InChI=1S/C15H24/c1-8(2)9-5-6-14(3)10-7-11-13(12(9)10)15(11,14)4/h8-13H,5-7H2,1-4H
InchiKey: XBWACJDEQIZTPR-UHFFFAOYSA-N
Formula: C15H24
SMILES: CC(C)C1CCC2(C)C3CC4C(C13)C42C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	306.07	kJ/mol	Joback Method
hf	-85.23	kJ/mol	Joback Method
hfus	18.44	kJ/mol	Joback Method
hvap	44.67	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.961		Crippen Method
mcvol	178.770	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1363.00		NIST Webbook
ripol	1492.00		NIST Webbook
ripol	1492.00		NIST Webbook
tb	547.05	K	Joback Method
tc	759.24	K	Joback Method
tf	357.69	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.57	J/mol×K	547.05	Joback Method
cpg	526.02	J/mol×K	582.42	Joback Method
cpg	546.77	J/mol×K	617.78	Joback Method
cpg	566.10	J/mol×K	653.15	Joback Method
cpg	584.32	J/mol×K	688.51	Joback Method
cpg	601.73	J/mol×K	723.88	Joback Method
cpg	618.64	J/mol×K	759.24	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=R600334&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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