Italicene

Inchi: InChI=1S/C15H24/c1-10-7-8-15-11(2)5-6-12(15)14(3,4)13(15)9-10/h9,11-13H,5-8H2,1-4
InchiKey: BWAXOYJGXIEEOE-UHFFFAOYSA-N
Formula: C15H24
SMILES: CC1=CC2C(C)(C)C3CCC(C)C23CC1
Mol. weight [g/mol]: 204.35
CAS: 94535-52-1

Physical Properties

Property code	Value	Unit	Source
gf	227.40	kJ/mol	Joback Method
hf	-110.74	kJ/mol	Joback Method
hfus	15.19	kJ/mol	Joback Method
hvap	47.10	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1404.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1400.00		NIST Webbook

rinpol	1407.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1414.60		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1400.00		NIST Webbook
ripol	1536.00		NIST Webbook
ripol	1517.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1489.00		NIST Webbook
ripol	1536.00		NIST Webbook
ripol	1542.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1536.00		NIST Webbook
tb	566.64	K	Joback Method
tc	792.17	K	Joback Method
tf	358.19	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.55	J/mol×K	566.64	Joback Method
cpg	526.55	J/mol×K	604.23	Joback Method
cpg	547.97	J/mol×K	641.82	Joback Method
cpg	568.10	J/mol×K	679.41	Joback Method
cpg	587.25	J/mol×K	716.99	Joback Method
cpg	605.70	J/mol×K	754.58	Joback Method
cpg	623.74	J/mol×K	792.17	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94535521&Units=SI

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