Isoitalicene

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-ABHRYQDASA-N
Formula: C15H24
SMILES: CC1=CC2C(C)(C)C3CCC(C)C23CC1
Mol. weight [g/mol]: 204.35
CAS: 94482-89-0

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	1398.00		NIST Webbook
rinpol	1384.80		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1376.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1475.00		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=C94482890&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