

Isocomene

Inchi: InChI=1S/C15H24/c1-11-6-9-14(4)12(2)10-13(3)7-5-8-15(11,13)14/h10-11H,5-9H2,1-4H3
InchiKey: SAOJPWFHRMUCFN-UQOMUDLDSA-N
Formula: C15H24
SMILES: CC1=CC2(C)CCCC23C(C)CCC13C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	229.62	kJ/mol	Joback Method
hf	-75.16	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	46.26	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	1392.00		NIST Webbook
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tb	571.55	K	Joback Method
tc	806.48	K	Joback Method
tf	386.33	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.53	J/molxK	571.55	Joback Method
cpg	523.86	J/molxK	610.71	Joback Method
cpg	544.56	J/molxK	649.86	Joback Method
cpg	564.09	J/molxK	689.02	Joback Method
cpg	582.88	J/molxK	728.17	Joback Method
cpg	601.40	J/molxK	767.33	Joback Method
cpg	620.08	J/molxK	806.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R604287&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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