«beta»-Humulene

Inchi: InChI=1S/C15H24/c1-13-7-5-8-14(2)10-12-15(3,4)11-6-9-13/h6,10-11H,1,5,7-9,12H2,2-4
InchiKey: HAVYZKHVTLAPDZ-PPGMXFKZSA-N
Formula: C15H24
SMILES: C=C1CC=CC(C)(C)CC=C(C)CCC1
Mol. weight [g/mol]: 204.35
CAS: 116-04-1

Physical Properties

Property code	Value	Unit	Source
gf	137.25	kJ/mol	Joback Method
hf	-125.84	kJ/mol	Joback Method
hfus	10.54	kJ/mol	Joback Method
hvap	50.53	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.035		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1453.50		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1454.00		NIST Webbook

rinpol	1453.50		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1454.00		NIST Webbook
ripol	1674.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1674.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1654.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1689.00		NIST Webbook
ripol	1654.00		NIST Webbook
ripol	1675.00		NIST Webbook
tb	586.20	K	Joback Method
tc	821.65	K	Joback Method
tf	300.21	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.47	J/mol×K	586.20	Joback Method
cpg	523.64	J/mol×K	625.44	Joback Method
cpg	546.38	J/mol×K	664.68	Joback Method
cpg	567.79	J/mol×K	703.92	Joback Method
cpg	587.97	J/mol×K	743.17	Joback Method
cpg	607.03	J/mol×K	782.41	Joback Method
cpg	625.07	J/mol×K	821.65	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116041&Units=SI

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

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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