«gamma»-Elemene

Inchi: InChI=1S/C15H24/c1-7-15(6)9-8-13(11(2)3)10-14(15)12(4)5/h7,14H,1,4,8-10H2,2-3,5-6H
InchiKey: BQSLMQNYHVFRDT-CABCVRRESA-N
Formula: C15H24
SMILES: C=CC1(C)CCC(=C(C)C)CC1C(=C)C
Mol. weight [g/mol]: 204.35
CAS: 30824-67-0

Physical Properties

Property code	Value	Unit	Source
gf	290.71	kJ/mol	Joback Method
hf	3.60	kJ/mol	Joback Method
hfus	16.36	kJ/mol	Joback Method
hvap	47.56	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.891		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1437.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1427.00		NIST Webbook

rinpol	1409.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1433.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1650.00		NIST Webbook
tb	557.48	K	Joback Method
tc	771.21	K	Joback Method
tf	264.77	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.96	J/mol×K	557.48	Joback Method
cpg	512.54	J/mol×K	593.10	Joback Method
cpg	532.84	J/mol×K	628.72	Joback Method
cpg	551.99	J/mol×K	664.35	Joback Method
cpg	570.13	J/mol×K	699.97	Joback Method
cpg	587.38	J/mol×K	735.59	Joback Method
cpg	603.88	J/mol×K	771.21	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=C30824670&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

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