B-Ionene

Inchi: InChI=1S/C13H20/c1-5-6-9-12-11(2)8-7-10-13(12,3)4/h5-6,9H,1,7-8,10H2,2-4H3/b9-6+
InchiKey: BWPHCNAZKLXPHW-RMKNXTFCSA-N
Formula: C13H20
SMILES: C=CC=CC1=C(C)CCCC1(C)C
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	256.30	kJ/mol	Joback Method
hf	35.40	kJ/mol	Joback Method
hfus	14.33	kJ/mol	Joback Method
hvap	44.71	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.255		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1483.00		NIST Webbook
tb	526.59	K	Joback Method
tc	742.08	K	Joback Method
tf	286.51	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.05	J/mol×K	526.59	Joback Method
cpg	411.99	J/mol×K	562.50	Joback Method
cpg	429.74	J/mol×K	598.42	Joback Method
cpg	446.43	J/mol×K	634.33	Joback Method
cpg	462.18	J/mol×K	670.25	Joback Method
cpg	477.13	J/mol×K	706.16	Joback Method
cpg	491.40	J/mol×K	742.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R292725&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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