Caparratriene

Other names: Capparatriene
Inchi: InChI=1S/C15H26/c1-6-14(4)10-8-12-15(5)11-7-9-13(2)3/h6,8-10,15H,7,11-12H2,1-5H3/
InchiKey: GIBJEWOSWWYJSK-CKGOAGCQSA-N
Formula: C15H26
SMILES: CC=C(C)C=CCC(C)CCC=C(C)C
Mol. weight [g/mol]: 206.37

Physical Properties

Property code	Value	Unit	Source
gf	296.54	kJ/mol	Joback Method
hf	-26.13	kJ/mol	Joback Method
hfus	29.07	kJ/mol	Joback Method
hvap	48.63	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	5.281		Crippen Method
mcvol	209.310	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	1493.00		NIST Webbook
ripol	1692.00		NIST Webbook
ripol	1692.00		NIST Webbook
tb	554.40	K	Joback Method
tc	742.01	K	Joback Method
tf	200.65	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.36	J/mol×K	554.40	Joback Method
cpg	523.14	J/mol×K	585.67	Joback Method
cpg	540.94	J/mol×K	616.94	Joback Method
cpg	557.82	J/mol×K	648.20	Joback Method
cpg	573.83	J/mol×K	679.47	Joback Method
cpg	589.03	J/mol×K	710.74	Joback Method

cpg	603.48	J/mol×K	742.01	Joback Method

Sources

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=U374087&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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