cis-Calamenene

Inchi: InChI=1S/C15H22/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5,7,9-10,12-13H,6,8H2,
InchiKey: PGTJIOWQJWHTJJ-STQMWFEESA-N
Formula: C15H22
SMILES: Cc1ccc2c(c1)C(C(C)C)CCC2C
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	207.07	kJ/mol	Joback Method
hf	-98.32	kJ/mol	Joback Method
hfus	21.45	kJ/mol	Joback Method
hvap	51.97	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.632		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1540.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1555.00		NIST Webbook
ripol	1839.00		NIST Webbook
ripol	1839.00		NIST Webbook
tb	585.14	K	Joback Method
tc	803.63	K	Joback Method
tf	305.45	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.92	J/mol×K	585.14	Joback Method
cpg	575.50	J/mol×K	767.21	Joback Method
cpg	559.26	J/mol×K	730.80	Joback Method
cpg	541.93	J/mol×K	694.38	Joback Method
cpg	523.46	J/mol×K	657.97	Joback Method
cpg	503.81	J/mol×K	621.55	Joback Method
cpg	590.72	J/mol×K	803.63	Joback Method
dvisc	0.0003052	Pa×s	585.14	Joback Method
dvisc	0.0003614	Pa×s	538.52	Joback Method
dvisc	0.0004418	Pa×s	491.91	Joback Method
dvisc	0.0005632	Pa×s	445.30	Joback Method
dvisc	0.0007601	Pa×s	398.68	Joback Method
dvisc	0.0011104	Pa×s	352.07	Joback Method
dvisc	0.0018212	Pa×s	305.45	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=R600314&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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