calamenene (1-S,cis)

Other names: 1S-cis-1,2,3,4-Tetrahydro-1,6-dimethyl-4-isopropylnaphthalene
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	1526.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1496.00		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	503.81	J/mol×K	621.55	Joback Method
cpg	523.46	J/mol×K	657.97	Joback Method
cpg	541.93	J/mol×K	694.38	Joback Method
cpg	559.26	J/mol×K	730.80	Joback Method
cpg	575.50	J/mol×K	767.21	Joback Method

cpg	590.72	J/mol×K	803.63	Joback Method
dvisc	0.0018212	Pa×s	305.45	Joback Method
dvisc	0.0011104	Pa×s	352.07	Joback Method
dvisc	0.0007601	Pa×s	398.68	Joback Method
dvisc	0.0005632	Pa×s	445.30	Joback Method
dvisc	0.0004418	Pa×s	491.91	Joback Method
dvisc	0.0003614	Pa×s	538.52	Joback Method
dvisc	0.0003052	Pa×s	585.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R237397&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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