

(E)-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-OLZOCXBDSA-N
Formula:	C15H22
SMILES:	<chem>Cc1ccc2c(c1)C(C(C)C)CCC2C</chem>
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	1516.00		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/molxK	585.14	Joback Method
cpg	503.81	J/molxK	621.55	Joback Method
cpg	523.46	J/molxK	657.97	Joback Method
cpg	541.93	J/molxK	694.38	Joback Method
cpg	559.26	J/molxK	730.80	Joback Method
cpg	575.50	J/molxK	767.21	Joback Method
cpg	590.72	J/molxK	803.63	Joback Method
dvisc	0.0018212	Paxs	305.45	Joback Method
dvisc	0.0011104	Paxs	352.07	Joback Method

dvisc	0.0007601	Paxs	398.68	Joback Method
dvisc	0.0005632	Paxs	445.30	Joback Method
dvisc	0.0004418	Paxs	491.91	Joback Method
dvisc	0.0003614	Paxs	538.52	Joback Method
dvisc	0.0003052	Paxs	585.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R616889&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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