

«sigma»-Cadinene

Inchi:	InChI=1S/C15H24/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h9-10,13,15H,5-8H2,1-4H
InchiKey:	FUCYIEXQVQJBKY-ZFWWWQNUSA-N
Formula:	C15H24
SMILES:	CC1=CC2C(=C(C)CCC2C(C)C)CC1
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	177.11	kJ/mol	Joback Method
hf	-156.10	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	51.68	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1523.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1530.50		NIST Webbook
rinpol	1524.00		NIST Webbook
ripol	1749.00		NIST Webbook
tb	585.98	K	Joback Method
tc	802.43	K	Joback Method
tf	304.69	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.23	J/mol×K	585.98	Joback Method
cpg	525.21	J/mol×K	622.06	Joback Method
cpg	545.92	J/mol×K	658.13	Joback Method
cpg	565.40	J/mol×K	694.21	Joback Method

cpg	583.72	J/mol×K	730.28	Joback Method
cpg	600.91	J/mol×K	766.36	Joback Method
cpg	617.03	J/mol×K	802.43	Joback Method
dvisc	0.0020981	Pa×s	304.69	Joback Method
dvisc	0.0012209	Pa×s	351.57	Joback Method
dvisc	0.0008070	Pa×s	398.45	Joback Method
dvisc	0.0005820	Pa×s	445.34	Joback Method
dvisc	0.0004467	Pa×s	492.22	Joback Method
dvisc	0.0003590	Pa×s	539.10	Joback Method
dvisc	0.0002988	Pa×s	585.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R281493&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

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

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