

Calacorene

Other names:	dihydro-1,6-dimethyl-4-(1-methylethyl)naphthalene
Inchi:	InChI=1S/C15H20/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5,7-10,12H,6H2,1-4H3
InchiKey:	YLIAZCIBLKJTKN-UHFFFAOYSA-N
Formula:	C15H20
SMILES:	<chem>Cc1ccc2c(c1)C(C(C)C)=CCC2C</chem>
Mol. weight [g/mol]:	200.32
CAS:	38599-17-6

Physical Properties

Property code	Value	Unit	Source
gf	235.11	kJ/mol	Joback Method
hf	-31.67	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	53.23	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.542		Crippen Method
mcvol	183.290	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1565.00		NIST Webbook

ripol	1538.00		NIST Webbook
ripol	1541.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1532.00		NIST Webbook
ripol	1916.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1918.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1916.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1916.00		NIST Webbook
ripol	1916.00		NIST Webbook
ripol	1916.00		NIST Webbook
ripol	1917.00		NIST Webbook
ripol	1916.00		NIST Webbook
tb	593.95	K	Joback Method
tc	815.53	K	Joback Method
tf	322.97	K	Joback Method
vc	0.697	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.53	J/molxK	593.95	Joback Method
cpg	480.53	J/molxK	630.88	Joback Method
cpg	498.37	J/molxK	667.81	Joback Method
cpg	515.11	J/molxK	704.74	Joback Method
cpg	530.81	J/molxK	741.67	Joback Method
cpg	545.52	J/molxK	778.60	Joback Method
cpg	559.31	J/molxK	815.53	Joback Method
dvisc	0.0015769	Paxs	322.97	Joback Method
dvisc	0.0009838	Paxs	368.13	Joback Method
dvisc	0.0006804	Paxs	413.30	Joback Method
dvisc	0.0005061	Paxs	458.46	Joback Method

dvisc	0.0003969	Paxs	503.62	Joback Method
dvisc	0.0003240	Paxs	548.79	Joback Method
dvisc	0.0002728	Paxs	593.95	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=C38599176&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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