«alpha»-Corocalene

Inchi:	InChI=1S/C15H20/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h6,8-10H,5,7H2,1-4H3
InchiKey:	VTUZIFHLLUSULC-UHFFFAOYSA-N
Formula:	C15H20
SMILES:	CC1=Cc2c(C(C)C)ccc(C)c2CC1
Mol. weight [g/mol]:	200.32
CAS:	20129-39-9

Physical Properties

Property code	Value	Unit	Source
gf	233.19	kJ/mol	Joback Method
hf	-22.80	kJ/mol	Joback Method
hfus	19.75	kJ/mol	Joback Method
hvap	54.21	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.468		Crippen Method
mcvol	183.290	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	1608.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1629.20		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1629.20		NIST Webbook
ripol	2060.00		NIST Webbook
ripol	2083.00		NIST Webbook
ripol	2037.00		NIST Webbook
tb	603.60	K	Joback Method
tc	826.16	K	Joback Method
tf	339.73	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.02	J/mol×K	603.60	Joback Method
cpg	540.71	J/mol×K	789.07	Joback Method
cpg	526.54	J/mol×K	751.98	Joback Method
cpg	511.45	J/mol×K	714.88	Joback Method
cpg	495.37	J/mol×K	677.79	Joback Method
cpg	478.25	J/mol×K	640.69	Joback Method
cpg	554.02	J/mol×K	826.16	Joback Method
dvisc	0.0002364	Pa×s	603.60	Joback Method
dvisc	0.0002851	Pa×s	559.62	Joback Method
dvisc	0.0003550	Pa×s	515.64	Joback Method
dvisc	0.0004605	Pa×s	471.67	Joback Method
dvisc	0.0006301	Pa×s	427.69	Joback Method
dvisc	0.0009265	Pa×s	383.71	Joback Method
dvisc	0.0015052	Pa×s	339.73	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=C20129399&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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