«gamma»-Calacorene

Inchi: InChI=1S/C15H20/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5-10,12-13H,1-4H3
InchiKey: LCROQSRTEMTLQQ-UHFFFAOYSA-N
Formula: C15H20
SMILES: Cc1ccc2c(c1)C(C(C)C)C=CC2C
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
gf	237.03	kJ/mol	Joback Method
hf	-40.54	kJ/mol	Joback Method
hfus	22.67	kJ/mol	Joback Method
hvap	52.26	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.408		Crippen Method
mcvol	183.290	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	1553.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1558.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1571.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
tb	584.30	K	Joback Method
tc	804.86	K	Joback Method

tf	306.21	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.66	J/mol×K	584.30	Joback Method
cpg	482.45	J/mol×K	621.06	Joback Method
cpg	501.03	J/mol×K	657.82	Joback Method
cpg	518.45	J/mol×K	694.58	Joback Method
cpg	534.78	J/mol×K	731.34	Joback Method
cpg	550.06	J/mol×K	768.10	Joback Method
cpg	564.36	J/mol×K	804.86	Joback Method
dvisc	0.0015832	Pa×s	306.21	Joback Method
dvisc	0.0010106	Pa×s	352.56	Joback Method
dvisc	0.0007160	Pa×s	398.91	Joback Method
dvisc	0.0005450	Pa×s	445.25	Joback Method
dvisc	0.0004368	Pa×s	491.60	Joback Method
dvisc	0.0003637	Pa×s	537.95	Joback Method
dvisc	0.0003117	Pa×s	584.30	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R237233&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