«beta»-Calacorene

Other names: Calacorene B
Inchi: InChI=1S/C15H20/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5,7,9-10,13H,4,6,8H2,1
InchiKey: KFYISTOZYAKAPV-UHFFFAOYSA-N
Formula: C15H20
SMILES: C=C1CCC(C(C)C)c2cc(C)ccc21
Mol. weight [g/mol]: 200.32
CAS: 50277-34-4

Physical Properties

Property code	Value	Unit	Source
gf	267.86	kJ/mol	Joback Method
hf	6.26	kJ/mol	Joback Method
hfus	19.22	kJ/mol	Joback Method
hvap	52.44	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.542		Crippen Method
mcvol	183.290	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	1565.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1548.00		NIST Webbook
rinpol	1552.00		NIST Webbook
rinpol	1552.00		NIST Webbook
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ripol	1979.00	NIST Webbook
ripol	1916.00	NIST Webbook
ripol	1918.00	NIST Webbook
ripol	1918.00	NIST Webbook
ripol	1918.00	NIST Webbook
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ripol	1955.00		NIST Webbook
ripol	1931.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1942.00		NIST Webbook
ripol	1913.00		NIST Webbook
ripol	1935.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1939.00		NIST Webbook
ripol	1932.00		NIST Webbook
tb	588.97	K	Joback Method
tc	809.35	K	Joback Method
tf	323.37	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.57	J/mol×K	588.97	Joback Method
cpg	545.53	J/mol×K	772.62	Joback Method
cpg	530.64	J/mol×K	735.89	Joback Method
cpg	514.76	J/mol×K	699.16	Joback Method
cpg	497.82	J/mol×K	662.43	Joback Method
cpg	479.77	J/mol×K	625.70	Joback Method
cpg	559.47	J/mol×K	809.35	Joback Method
dvisc	0.0002992	Pa×s	588.97	Joback Method
dvisc	0.0003549	Pa×s	544.70	Joback Method
dvisc	0.0004338	Pa×s	500.44	Joback Method
dvisc	0.0005514	Pa×s	456.17	Joback Method
dvisc	0.0007379	Pa×s	411.90	Joback Method
dvisc	0.0010592	Pa×s	367.64	Joback Method
dvisc	0.0016787	Pa×s	323.37	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=C50277344&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