«beta»-Calacorene

Inchi: InChI=1S/C15H20/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5,7,9,12H,6,8H2,1-4H3
InchiKey: HDBSITBZJGRUAD-UHFFFAOYSA-N
Formula: C15H20
SMILES: CC(C)=C1CCC(C)c2ccc(C)cc21
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
gf	254.13	kJ/mol	Joback Method
hf	-6.46	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hvap	53.54	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.686		Crippen Method
mcvol	183.290	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1565.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1566.00		NIST Webbook
ripol	1942.00		NIST Webbook
tb	596.77	K	Joback Method
tc	821.36	K	Joback Method
tf	321.09	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.34	J/mol×K	596.77	Joback Method
cpg	480.53	J/mol×K	634.20	Joback Method
cpg	498.53	J/mol×K	671.63	Joback Method
cpg	515.41	J/mol×K	709.06	Joback Method
cpg	531.24	J/mol×K	746.49	Joback Method
cpg	546.07	J/mol×K	783.93	Joback Method
cpg	559.99	J/mol×K	821.36	Joback Method

Sources

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=R604836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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