«alpha»-Vetispirene

Inchi: InChI=1S/C15H22/c1-11(2)14-8-9-15(10-14)12(3)6-5-7-13(15)4/h6,10,13H,1,5,7-9H2,2-4
InchiKey: KEVTZKPBXQTBSV-UHFFFAOYSA-N
Formula: C15H22
SMILES: C=C(C)C1=CC2(CC1)C(C)=CCCC2C
Mol. weight [g/mol]: 202.34
CAS: 51196-11-3

Physical Properties

Property code	Value	Unit	Source
gf	262.98	kJ/mol	Joback Method
hf	-8.47	kJ/mol	Joback Method
hfus	15.25	kJ/mol	Joback Method
hvap	49.67	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.645		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1481.00		NIST Webbook
rinpol	1494.60		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1494.60		NIST Webbook
tb	578.24	K	Joback Method
tc	806.39	K	Joback Method
tf	315.35	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.59	J/mol×K	578.24	Joback Method
cpg	501.10	J/mol×K	616.26	Joback Method
cpg	521.21	J/mol×K	654.29	Joback Method
cpg	540.12	J/mol×K	692.31	Joback Method

cpg	557.97	J/mol×K	730.34	Joback Method
cpg	574.96	J/mol×K	768.36	Joback Method
cpg	591.25	J/mol×K	806.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51196113&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume