«alpha»-Pyrovetivene

Inchi: InChI=1S/C15H22/c1-11(2)13-8-9-14-7-5-6-12(3)15(14,4)10-13/h7-9,12H,5-6,10H2,1-4H
InchiKey: OGJMWHSJNRCMCN-SWLSCSKDSA-N
Formula: C15H22
SMILES: CC(C)=C1C=CC2=CCCC(C)C2(C)C1
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	230.23	kJ/mol	Joback Method
hf	-46.40	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	50.46	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.645		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1817.00		NIST Webbook
tb	583.22	K	Joback Method
tc	812.62	K	Joback Method
tf	314.95	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.83	J/mol×K	583.22	Joback Method
cpg	502.10	J/mol×K	621.45	Joback Method
cpg	522.00	J/mol×K	659.69	Joback Method
cpg	540.71	J/mol×K	697.92	Joback Method
cpg	558.40	J/mol×K	736.15	Joback Method

cpg	575.26	J/mol×K	774.38	Joback Method
cpg	591.45	J/mol×K	812.62	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R206932&Units=SI

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