«alpha»-Acoradiene

Inchi: InChI=1S/C15H24/c1-11(2)14-6-5-13(4)15(14)9-7-12(3)8-10-15/h6-7,9,11-13H,5,8,10H2,
InchiKey: XTISJFXWBIASHF-JVWICGRDSA-N
Formula: C15H24
SMILES: CC1C=CC2(CC1)C(C(C)C)=CCC2C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	183.17	kJ/mol	Joback Method
hf	-138.26	kJ/mol	Joback Method
hfus	15.78	kJ/mol	Joback Method
hvap	48.90	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1471.00		NIST Webbook

ripol	1690.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1690.00		NIST Webbook
tb	571.59	K	Joback Method
tc	794.61	K	Joback Method
tf	299.31	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.14	J/mol×K	571.59	Joback Method
cpg	524.19	J/mol×K	608.76	Joback Method
cpg	545.79	J/mol×K	645.93	Joback Method
cpg	566.10	J/mol×K	683.10	Joback Method
cpg	585.27	J/mol×K	720.27	Joback Method
cpg	603.45	J/mol×K	757.44	Joback Method
cpg	620.81	J/mol×K	794.61	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=R232194&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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