undulatene

Other names: (-)-Perfora-1,7-diene
Inchi: InChI=1S/C15H24/c1-11-5-8-14-12(2)6-7-13(3)15(14,4)10-9-11/h6,9,13-14H,5,7-8,10H2,
InchiKey: NZAPWYHXDQNUKG-LOWNFYCTSA-N
Formula: C15H24
SMILES: CC1=CCC2(C)C(C)CC=C(C)C2CC1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	163.88	kJ/mol	Joback Method
hf	-150.61	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	50.12	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1543.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1543.00		NIST Webbook
ripol	1812.00		NIST Webbook
ripol	1812.00		NIST Webbook
ripol	1812.00		NIST Webbook
tb	581.28	K	Joback Method
tc	808.29	K	Joback Method
tf	323.31	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.31	J/mol×K	581.28	Joback Method
cpg	526.59	J/mol×K	619.11	Joback Method
cpg	548.47	J/mol×K	656.95	Joback Method

cpg	569.08	J/mol×K	694.78	Joback Method
cpg	588.58	J/mol×K	732.62	Joback Method
cpg	607.10	J/mol×K	770.45	Joback Method
cpg	624.78	J/mol×K	808.29	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=R141741&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