«alpha»-pseudowiddrene

Other names: Pseudowiddrene
Inchi: InChI=1S/C15H24/c1-12-7-8-13-6-5-10-14(2,3)15(13,4)11-9-12/h6,9H,5,7-8,10-11H2,1-4
InchiKey: HIGJBMFZAPBLEG-HNNXBMFYSA-N
Formula: C15H24
SMILES: CC1=CCC2(C)C(=CCCC2(C)C)CC1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	166.10	kJ/mol	Joback Method
hf	-115.03	kJ/mol	Joback Method
hfus	9.45	kJ/mol	Joback Method
hvap	49.28	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1523.00		NIST Webbook
rinpol	1523.00		NIST Webbook
ripol	1745.00		NIST Webbook
tb	586.19	K	Joback Method
tc	822.53	K	Joback Method
tf	351.45	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.78	J/mol×K	586.19	Joback Method
cpg	523.43	J/mol×K	625.58	Joback Method
cpg	544.65	J/mol×K	664.97	Joback Method
cpg	564.73	J/mol×K	704.36	Joback Method
cpg	583.94	J/mol×K	743.75	Joback Method
cpg	602.58	J/mol×K	783.14	Joback Method

cpg	620.93	J/mol×K	822.53	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=R338891&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