Isogermacrene D

Inchi: InChI=1S/C15H24/c1-12(2)15-10-8-13(3)6-5-7-14(4)9-11-15/h7-8,10,12,15H,3,5-6,9,11H
InchiKey: GAIBLDCXCZKKJE-ACWLMNNXSA-N
Formula: C15H24
SMILES: C=C1C=CC(C(C)C)CCC(C)=CCC1
Mol. weight [g/mol]: 204.35
CAS: 317819-80-0

Physical Properties

Property code	Value	Unit	Source
gf	152.40	kJ/mol	Joback Method
hf	-140.20	kJ/mol	Joback Method
hfus	15.41	kJ/mol	Joback Method
hvap	51.12	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.891		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1445.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1431.00		NIST Webbook
ripol	1665.00		NIST Webbook
tb	581.25	K	Joback Method
tc	804.50	K	Joback Method
tf	264.83	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	499.53	J/mol×K	581.25	Joback Method
cpg	523.14	J/mol×K	618.46	Joback Method
cpg	545.41	J/mol×K	655.67	Joback Method
cpg	566.34	J/mol×K	692.88	Joback Method
cpg	585.93	J/mol×K	730.09	Joback Method
cpg	604.19	J/mol×K	767.29	Joback Method
cpg	621.12	J/mol×K	804.50	Joback Method
dvisc	0.0085131	Pa×s	264.83	Joback Method
dvisc	0.0019587	Pa×s	317.57	Joback Method
dvisc	0.0006848	Pa×s	370.30	Joback Method
dvisc	0.0003112	Pa×s	423.04	Joback Method
dvisc	0.0001684	Pa×s	475.78	Joback Method
dvisc	0.0001030	Pa×s	528.51	Joback Method
dvisc	0.0000689	Pa×s	581.25	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C317819800&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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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