Isogermacrene D

Inchi: InChI=1S/C16H26/c1-13(2)16-10-6-9-14(3)7-5-8-15(4)11-12-16/h6,8-9,13,16H,3,5,7,10-1
InchiKey: NDKRHWBZQMLINJ-DPFABPHNSA-N
Formula: C16H26
SMILES: C=C1C=CCC(C(C)C)CCC(C)=CCC1
Mol. weight [g/mol]: 218.38

Physical Properties

Property code	Value	Unit	Source
gf	148.72	kJ/mol	Joback Method
hf	-167.00	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	53.52	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.281		Crippen Method
mcvol	212.540	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	1385.00		NIST Webbook
tb	608.40	K	Joback Method
tc	835.10	K	Joback Method
tf	272.58	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.80	J/mol×K	608.40	Joback Method
cpg	665.81	J/mol×K	797.31	Joback Method
cpg	646.82	J/mol×K	759.53	Joback Method
cpg	626.33	J/mol×K	721.75	Joback Method
cpg	604.33	J/mol×K	683.97	Joback Method
cpg	580.82	J/mol×K	646.18	Joback Method
cpg	683.27	J/mol×K	835.10	Joback Method
dvisc	0.0000459	Pa×s	608.40	Joback Method
dvisc	0.0000714	Pa×s	552.43	Joback Method

dvisc	0.0001226	Pa×s	496.46	Joback Method
dvisc	0.0002416	Pa×s	440.49	Joback Method
dvisc	0.0005802	Pa×s	384.52	Joback Method
dvisc	0.0018776	Pa×s	328.55	Joback Method
dvisc	0.0098418	Pa×s	272.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630914&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume