Isogermacrene

Inchi: InChI=1S/C15H24/c1-12(2)15-10-6-8-13(3)7-5-9-14(4)11-15/h7,11,15H,1,5-6,8-10H2,2-4
InchiKey: YSOYXLPARMWZFY-WYBATKFCSA-N
Formula: C15H24
SMILES: C=C(C)C1C=C(C)CCC=C(C)CCC1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	171.42	kJ/mol	Joback Method
hf	-114.99	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.035		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1446.00		NIST Webbook
tb	584.07	K	Joback Method
tc	810.41	K	Joback Method
tf	262.95	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.67	J/mol×K	584.07	Joback Method
cpg	523.53	J/mol×K	621.79	Joback Method
cpg	546.01	J/mol×K	659.52	Joback Method
cpg	567.11	J/mol×K	697.24	Joback Method
cpg	586.84	J/mol×K	734.97	Joback Method
cpg	605.21	J/mol×K	772.69	Joback Method
cpg	622.25	J/mol×K	810.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R416738&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
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

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