

Germacrane-d

Inchi:	InChI=1S/C15H30/c1-12(2)15-10-8-13(3)6-5-7-14(4)9-11-15/h12-15H,5-11H2,1-4H3
InchiKey:	IBMAYSYZAVZPY-UHFFFAOYSA-N
Formula:	C15H30
SMILES:	CC1CCCC(C)CCC(C(C)C)CC1
Mol. weight [g/mol]:	210.40

Physical Properties

Property code	Value	Unit	Source
gf	33.61	kJ/mol	Joback Method
hf	-369.21	kJ/mol	Joback Method
hfus	16.66	kJ/mol	Joback Method
hvap	49.09	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	5.275		Crippen Method
mcvol	211.350	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	1485.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1489.00		NIST Webbook
tb	569.45	K	Joback Method
tc	785.52	K	Joback Method
tf	228.63	K	Joback Method
vc	0.768	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.87	J/mol×K	569.45	Joback Method
cpg	588.12	J/mol×K	605.46	Joback Method
cpg	614.87	J/mol×K	641.47	Joback Method
cpg	640.11	J/mol×K	677.48	Joback Method

cpg	663.85	J/molxK	713.49	Joback Method
cpg	686.09	J/molxK	749.51	Joback Method
cpg	706.83	J/molxK	785.52	Joback Method
dvisc	0.0283190	Paxs	228.63	Joback Method
dvisc	0.0040194	Paxs	285.43	Joback Method
dvisc	0.0010907	Paxs	342.24	Joback Method
dvisc	0.0004291	Paxs	399.04	Joback Method
dvisc	0.0002130	Paxs	455.84	Joback Method
dvisc	0.0001235	Paxs	512.65	Joback Method
dvisc	0.0000798	Paxs	569.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R289640&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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