

Thunbergol

Other names:	(1R,2E,4S,7E,11E)-4-Isopropyl-1,7,11-trimethylcyclotetradeca-2,7,11-trienol Isocembrol
Inchi:	InChI=1S/C20H34O/c1-16(2)19-12-11-18(4)9-6-8-17(3)10-7-14-20(5,21)15-13-19/h9-10,
InchiKey:	YAPXSYXFLHDPCK-MAUDFNNOSA-N
Formula:	C20H34O
SMILES:	<chem>CC1=CCCC(C)(O)C=CC(C(C)C)CCC(C)=CCC1</chem>
Mol. weight [g/mol]:	290.48
CAS:	25269-17-4

Physical Properties

Property code	Value	Unit	Source
gf	-36.67	kJ/mol	Joback Method
hf	-463.30	kJ/mol	Joback Method
hfus	20.82	kJ/mol	Joback Method
hvap	78.95	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.813		Crippen Method
mcvol	274.770	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	2047.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2073.00		NIST Webbook
rinpol	2094.00		NIST Webbook
rinpol	2032.00		NIST Webbook
ripol	2575.00		NIST Webbook
ripol	2498.00		NIST Webbook
ripol	2575.00		NIST Webbook
tb	805.46	K	Joback Method
tc	1028.60	K	Joback Method
tf	387.18	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.52	J/mol×K	805.46	Joback Method
cpg	900.62	J/mol×K	842.65	Joback Method
cpg	922.31	J/mol×K	879.84	Joback Method
cpg	942.67	J/mol×K	917.03	Joback Method
cpg	961.78	J/mol×K	954.22	Joback Method
cpg	979.69	J/mol×K	991.41	Joback Method
cpg	996.50	J/mol×K	1028.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25269174&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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