(E)-«gamma»-Bisabolene

Other names:	trans-«gamma»-Bisabolene
	«gamma»-E-Bisabolene
Inchi:	InChI=1S/C15H24/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h6,8H,5,7,9-11H2,1-4H3/b1
InchiKey:	XBGUIVFBMBVUEG-PFONDFGASA-N
Formula:	C15H24
SMILES:	CC(C)=CCCC(C)=C1CC=C(C)CC1
Mol. weight [g/mol]:	204.35
CAS:	53585-13-0

Physical Properties

Property code	Value	Unit	Source
gf	236.49	kJ/mol	Joback Method
hf	-58.29	kJ/mol	Joback Method
hfus	24.11	kJ/mol	Joback Method
hvap	51.58	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.179		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	1530.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1538.40		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1533.00		NIST Webbook
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ripol	1727.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1766.00		NIST Webbook
ripol	1761.00		NIST Webbook
tb	581.52	K	Joback Method
tc	790.68	K	Joback Method
tf	261.07	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.12	J/mol×K	581.52	Joback Method
cpg	514.12	J/mol×K	616.38	Joback Method
cpg	532.97	J/mol×K	651.24	Joback Method
cpg	550.75	J/mol×K	686.10	Joback Method
cpg	567.52	J/mol×K	720.96	Joback Method
cpg	583.32	J/mol×K	755.82	Joback Method
cpg	598.22	J/mol×K	790.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53585130&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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