

(Z)-«alpha»-Santalol

Inchi: InChI=1S/C16H26O/c1-10(9-17)5-4-6-11(2)15-12-7-13-14(8-12)16(13,15)3/h5,11-15,17H
InchiKey: UWSUGXFVYBVFDX-OPAXWRLRSA-N
Formula: C16H26O
SMILES: CC(=CCCC(C)C1C2CC3C(C2)C31C)CO
Mol. weight [g/mol]: 234.38

Physical Properties

Property code	Value	Unit	Source
gf	201.79	kJ/mol	Joback Method
hf	-218.37	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	65.17	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.633		Crippen Method
mcvol	205.290	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1679.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1667.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2316.00		NIST Webbook
tb	663.84	K	Joback Method

tc	852.58	K	Joback Method
tf	373.14	K	Joback Method
vc	0.808	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.77	J/mol×K	663.84	Joback Method
cpg	640.87	J/mol×K	695.30	Joback Method
cpg	657.19	J/mol×K	726.75	Joback Method
cpg	672.89	J/mol×K	758.21	Joback Method
cpg	688.11	J/mol×K	789.67	Joback Method
cpg	703.02	J/mol×K	821.12	Joback Method
cpg	717.77	J/mol×K	852.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R131541&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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