(E)-Sesquilavandulol

Other names: trans-Sesquilavandulol
Sesquilavandulol (E)
Inchi: InChI=1S/C15H26O/c1-12(2)7-6-8-14(5)9-10-15(11-16)13(3)4/h7,9,15-16H,3,6,8,10-11H
InchiKey: JTSPVWIYQLSMER-NTEUORMPSA-N
Formula: C15H26O
SMILES: C=C(C)C(CO)CC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 222.37
CAS: 120707-27-9

Physical Properties

Property code	Value	Unit	Source
gf	158.79	kJ/mol	Joback Method
hf	-179.94	kJ/mol	Joback Method
hfus	30.36	kJ/mol	Joback Method
hvap	64.76	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.254		Crippen Method
mcvol	215.180	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	1599.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1635.00		NIST Webbook
ripol	2183.00		NIST Webbook
ripol	2148.00		NIST Webbook
ripol	2148.00		NIST Webbook
ripol	2183.00		NIST Webbook
ripol	2183.00		NIST Webbook
ripol	2183.00		NIST Webbook

ripol	2183.00		NIST Webbook
tb	638.98	K	Joback Method
tc	817.59	K	Joback Method
tf	250.83	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.53	J/mol×K	638.98	Joback Method
cpg	588.24	J/mol×K	668.75	Joback Method
cpg	603.19	J/mol×K	698.52	Joback Method
cpg	617.41	J/mol×K	728.29	Joback Method
cpg	630.96	J/mol×K	758.06	Joback Method
cpg	643.89	J/mol×K	787.82	Joback Method
cpg	656.23	J/mol×K	817.59	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C120707279&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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