VERBENYL PROPYL ETHER

Other names: Verbenol propyl ether
Inchi: InChI=1S/C13H22O/c1-5-6-14-12-7-9(2)10-8-11(12)13(10,3)4/h7,10-12H,5-6,8H2,1-4H3
InchiKey: GREQYBWLTCPCAU-UHFFFAOYSA-N
Formula: C13H22O
SMILES: CCCOC1C=C(C)C2CC1C2(C)C
Mol. weight [g/mol]: 194.32

Physical Properties

Property code	Value	Unit	Source
hfus	21.46	kJ/mol	Joback Method
hvap	58.76	kJ/mol	Cheméo Relay (1.0)
logp	3.404		Crippen Method
mcvol	173.880	ml/mol	McGowan Method
rinpol	1302.00		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.22	J/mol×K	532.05	Joback Method
cpg	462.70	J/mol×K	565.20	Joback Method
cpg	481.09	J/mol×K	598.35	Joback Method
cpg	498.48	J/mol×K	631.50	Joback Method
cpg	515.00	J/mol×K	664.65	Joback Method
cpg	530.73	J/mol×K	697.80	Joback Method
cpg	545.79	J/mol×K	730.96	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U108772&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices