verbenyl ethyl ether

Other names: (1R,4S,5R)-4-Ethoxy-2,6,6-trimethylbicyclo[3.1.1]hept-2-ene
Inchi: InChI=1S/C12H20O/c1-5-13-11-6-8(2)9-7-10(11)12(9,3)4/h6,9-11H,5,7H2,1-4H3
InchiKey: LQQWUEVOGQWTBB-UHFFFAOYSA-N
Formula: C12H20O
SMILES: CCOC1C=C(C)C2CC1C2(C)C
Mol. weight [g/mol]: 180.29
CAS: 80581-06-2

Physical Properties

Property code	Value	Unit	Source
gf	53.98	kJ/mol	Joback Method
hf	-262.92	kJ/mol	Joback Method
hfus	18.87	kJ/mol	Joback Method
hvap	43.90	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	3.014		Crippen Method
mcvol	159.790	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1186.20		NIST Webbook
ripol	1382.00		NIST Webbook
tb	509.17	K	Joback Method
tc	710.88	K	Joback Method
tf	308.29	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.15	J/mol×K	509.17	Joback Method
cpg	413.12	J/mol×K	542.79	Joback Method
cpg	430.98	J/mol×K	576.41	Joback Method
cpg	447.82	J/mol×K	610.02	Joback Method
cpg	463.76	J/mol×K	643.64	Joback Method
cpg	478.89	J/mol×K	677.26	Joback Method

cpg	493.34	J/mol×K	710.88	Joback Method

Sources

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=C80581062&Units=SI
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
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