coniferyl ethyl ether

Inchi: InChI=1S/C12H16O3/c1-3-15-8-4-5-10-6-7-11(13)12(9-10)14-2/h4-7,9,13H,3,8H2,1-2H3/
InchiKey: FXTHXNMWVSIYKM-SNAWJCMRSA-N
Formula: C12H16O3
SMILES: CCOCC=Cc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 208.25

Physical Properties

Property code	Value	Unit	Source
gf	-131.46	kJ/mol	Joback Method
hf	-390.48	kJ/mol	Joback Method
hfus	28.85	kJ/mol	Joback Method
hvap	63.04	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.450		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1730.00		NIST Webbook
rinpol	1730.00		NIST Webbook
tb	635.24	K	Joback Method
tc	851.23	K	Joback Method
tf	415.04	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.61	J/mol×K	635.24	Joback Method
cpg	448.45	J/mol×K	671.24	Joback Method
cpg	461.50	J/mol×K	707.24	Joback Method
cpg	473.83	J/mol×K	743.23	Joback Method
cpg	485.48	J/mol×K	779.23	Joback Method
cpg	496.53	J/mol×K	815.23	Joback Method
cpg	507.02	J/mol×K	851.23	Joback Method
dvisc	0.0004874	Pa×s	415.04	Joback Method

dvisc	0.0002161	Pa×s	451.74	Joback Method
dvisc	0.0001082	Pa×s	488.44	Joback Method
dvisc	0.0000597	Pa×s	525.14	Joback Method
dvisc	0.0000356	Pa×s	561.84	Joback Method
dvisc	0.0000226	Pa×s	598.54	Joback Method
dvisc	0.0000152	Pa×s	635.24	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R421062&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume