Coahuilensol, methyl ether (anisole, 2-ethenyl-3-methyl)

Inchi: InChI=1S/C10H12O/c1-4-9-8(2)6-5-7-10(9)11-3/h4-7H,1H2,2-3H3
InchiKey: CMKPBJQAYMKEON-UHFFFAOYSA-N
Formula: C10H12O
SMILES: C=Cc1c(C)cccc1OC
Mol. weight [g/mol]: 148.20

Physical Properties

Property code	Value	Unit	Source
gf	109.31	kJ/mol	Joback Method
hf	-42.93	kJ/mol	Joback Method
hfus	14.83	kJ/mol	Joback Method
hvap	43.19	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.647		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1222.00		NIST Webbook
rinpol	1222.00		NIST Webbook
tb	483.94	K	Joback Method
tc	694.09	K	Joback Method
tf	274.39	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.69	J/mol×K	483.94	Joback Method
cpg	277.90	J/mol×K	518.97	Joback Method
cpg	290.49	J/mol×K	553.99	Joback Method
cpg	302.46	J/mol×K	589.02	Joback Method
cpg	313.81	J/mol×K	624.04	Joback Method
cpg	324.57	J/mol×K	659.07	Joback Method
cpg	334.75	J/mol×K	694.09	Joback Method
dvisc	0.0012815	Pa×s	274.39	Joback Method

dvisc	0.0007693	Pa×s	309.31	Joback Method
dvisc	0.0005123	Pa×s	344.24	Joback Method
dvisc	0.0003676	Pa×s	379.16	Joback Method
dvisc	0.0002790	Pa×s	414.09	Joback Method
dvisc	0.0002211	Pa×s	449.01	Joback Method
dvisc	0.0001811	Pa×s	483.94	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=R568859&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