

Coahuilensol methyl ether

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	1196.00		NIST Webbook
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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/molxK	483.94	Joback Method
cpg	277.90	J/molxK	518.97	Joback Method
cpg	290.49	J/molxK	553.99	Joback Method
cpg	302.46	J/molxK	589.02	Joback Method
cpg	313.81	J/molxK	624.04	Joback Method
cpg	324.57	J/molxK	659.07	Joback Method
cpg	334.75	J/molxK	694.09	Joback Method
dvisc	0.0012815	Paxs	274.39	Joback Method

dvisc	0.0007693	Paxs	309.31	Joback Method
dvisc	0.0005123	Paxs	344.24	Joback Method
dvisc	0.0003676	Paxs	379.16	Joback Method
dvisc	0.0002790	Paxs	414.09	Joback Method
dvisc	0.0002211	Paxs	449.01	Joback Method
dvisc	0.0001811	Paxs	483.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R612149&Units=SI
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

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

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