

buta-1,3-dienyl methyl ether

Other names:	1-Methoxy-1,3-butadiene
Inchi:	InChI=1S/C5H8O/c1-3-4-5-6-2/h3-5H,1H2,2H3
InchiKey:	KOCUMXQOUWPSLK-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	C=CC=COC
Mol. weight [g/mol]:	84.12
CAS:	3036-66-6

Physical Properties

Property code	Value	Unit	Source
gf	54.28	kJ/mol	Joback Method
hf	-36.10	kJ/mol	Joback Method
hfus	8.82	kJ/mol	Joback Method
hvap	28.42	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	1.333		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
tb	364.70	K	NIST Webbook
tc	514.18	K	Joback Method
tf	214.40 ± 0.60	K	NIST Webbook
vc	0.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	121.28	J/mol×K	337.06	Joback Method
cpg	129.12	J/mol×K	366.58	Joback Method
cpg	136.65	J/mol×K	396.10	Joback Method
cpg	143.88	J/mol×K	425.62	Joback Method
cpg	150.81	J/mol×K	455.14	Joback Method
cpg	157.45	J/mol×K	484.66	Joback Method
cpg	163.82	J/mol×K	514.18	Joback Method
dvisc	0.0022496	Pa×s	161.50	Joback Method

dvisc	0.0010380	Pa×s	190.76	Joback Method
dvisc	0.0005883	Pa×s	220.02	Joback Method
dvisc	0.0003810	Pa×s	249.28	Joback Method
dvisc	0.0002703	Pa×s	278.54	Joback Method
dvisc	0.0002047	Pa×s	307.80	Joback Method
dvisc	0.0001627	Pa×s	337.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3036666&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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