

propargylethyl ether

Inchi:	InChI=1S/C5H8O/c1-3-5-6-4-2/h1H,4-5H2,2H3
InchiKey:	ADJMUEKUQLFLQP-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	C#CCOCC
Mol. weight [g/mol]:	84.12
CAS:	628-33-1

Physical Properties

Property code	Value	Unit	Source
gf	109.29	kJ/mol	Joback Method
hf	13.15	kJ/mol	Joback Method
hfus	12.87	kJ/mol	Joback Method
hvap	28.99	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.656		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
rinpol	571.00		NIST Webbook
rinpol	571.00		NIST Webbook
tb	326.34	K	Joback Method
tc	502.49	K	Joback Method
tf	215.31	K	Joback Method
vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	128.85	J/mol×K	326.34	Joback Method
cpg	135.75	J/mol×K	355.70	Joback Method
cpg	142.44	J/mol×K	385.06	Joback Method
cpg	148.93	J/mol×K	414.42	Joback Method
cpg	155.21	J/mol×K	443.77	Joback Method
cpg	161.30	J/mol×K	473.13	Joback Method
cpg	167.18	J/mol×K	502.49	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=C628331&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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