Propene-d6

Inchi: InChI=1S/C3H6/c1-3-2/h3H,1H2,2H3/i1D2,2D3,3D
InchiKey: QQONPFPTGQHPMA-QNYGJALNSA-N
Formula: C3D6
SMILES: C=CC
Mol. weight [g/mol]: 48.12
CAS: 1517-52-8

Physical Properties

Property code	Value	Unit	Source
gf	62.22	kJ/mol	Joback Method
hf	20.18	kJ/mol	Joback Method
hfus	2.25	kJ/mol	Joback Method
hvap	21.60	kJ/mol	Joback Method
ie	9.76 ± 0.01	eV	NIST Webbook
log10ws	-0.93		Crippen Method
logp	1.192		Crippen Method
mcvol	48.830	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
tb	264.72	K	Joback Method
tc	427.32	K	Joback Method
tf	121.81	K	Joback Method
vc	0.184	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	57.74	J/mol×K	264.72	Joback Method
cpg	62.84	J/mol×K	291.82	Joback Method
cpg	67.75	J/mol×K	318.92	Joback Method
cpg	72.49	J/mol×K	346.02	Joback Method
cpg	77.05	J/mol×K	373.12	Joback Method
cpg	81.45	J/mol×K	400.22	Joback Method
cpg	85.67	J/mol×K	427.32	Joback Method
dvisc	0.0013205	Pa×s	121.81	Joback Method

dvisc	0.0006501	Pa×s	145.63	Joback Method
dvisc	0.0003906	Pa×s	169.45	Joback Method
dvisc	0.0002661	Pa×s	193.27	Joback Method
dvisc	0.0001972	Pa×s	217.08	Joback Method
dvisc	0.0001551	Pa×s	240.90	Joback Method
dvisc	0.0001273	Pa×s	264.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1517528&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
ie:	Ionization energy
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