Propen-2-ol

Inchi: InChI=1S/C3H6O/c1-3(2)4/h4H,1H2,2H3
InchiKey: NARVIWMVBMUEOG-UHFFFAOYSA-N
Formula: C3H6O
SMILES: C=C(C)O
Mol. weight [g/mol]: 58.08
CAS: 74324-85-9

Physical Properties

Property code	Value	Unit	Source
gf	-83.15	kJ/mol	Joback Method
hf	-141.84	kJ/mol	Joback Method
hfus	5.02	kJ/mol	Joback Method
hvap	38.36	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	1.078		Crippen Method
mcvol	54.700	ml/mol	McGowan Method
pc	5351.35	kPa	Joback Method
rinpol	534.00		NIST Webbook
tb	356.78	K	Joback Method
tc	525.49	K	Joback Method
tf	168.67	K	Joback Method
vc	0.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	88.38	J/mol×K	356.78	Joback Method
cpg	93.45	J/mol×K	384.90	Joback Method
cpg	98.30	J/mol×K	413.02	Joback Method
cpg	102.96	J/mol×K	441.14	Joback Method
cpg	107.41	J/mol×K	469.26	Joback Method
cpg	111.68	J/mol×K	497.37	Joback Method
cpg	115.76	J/mol×K	525.49	Joback Method

Sources

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=C74324859&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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