3-Decyn-2-ol

Inchi: InChI=1S/C10H18O/c1-3-4-5-6-7-8-9-10(2)11/h10-11H,3-7H2,1-2H3
InchiKey: PGIQIBRWODQISW-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CCCCCCC#CC(C)O
Mol. weight [g/mol]: 154.25
CAS: 69668-93-5

Physical Properties

Property code	Value	Unit	Source
gf	96.86	kJ/mol	Joback Method
hf	-134.94	kJ/mol	Joback Method
hfus	25.34	kJ/mol	Joback Method
hvap	56.30	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.341		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	141.90		NIST Webbook
rinpol	160.50		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1101.00		NIST Webbook
tb	528.94	K	Joback Method
tc	708.63	K	Joback Method
tf	354.38	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.41	J/mol×K	528.94	Joback Method
cpg	359.20	J/mol×K	558.89	Joback Method
cpg	371.45	J/mol×K	588.84	Joback Method
cpg	383.18	J/mol×K	618.79	Joback Method
cpg	394.40	J/mol×K	648.74	Joback Method

cpg	405.12	J/mol×K	678.68	Joback Method
cpg	415.37	J/mol×K	708.63	Joback Method

Sources

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=C69668935&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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