9-Methylundec-1-en-3-ol

Inchi: InChI=1S/C12H24O/c1-4-11(3)9-7-6-8-10-12(13)5-2/h5,11-13H,2,4,6-10H2,1,3H3
InchiKey: XKVPGXANUNAWFV-UHFFFAOYSA-N
Formula: C12H24O
SMILES: C=CC(O)CCCCCC(C)CC
Mol. weight [g/mol]: 184.32

Physical Properties

Property code	Value	Unit	Source
gf	-3.70	kJ/mol	Joback Method
hf	-328.37	kJ/mol	Joback Method
hfus	22.60	kJ/mol	Joback Method
hvap	57.54	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.530		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1362.00		NIST Webbook
tb	561.94	K	Joback Method
tc	727.16	K	Joback Method
tf	254.06	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.71	J/mol×K	561.94	Joback Method
cpg	526.16	J/mol×K	699.62	Joback Method
cpg	513.83	J/mol×K	672.08	Joback Method
cpg	500.94	J/mol×K	644.55	Joback Method
cpg	487.47	J/mol×K	617.01	Joback Method
cpg	473.40	J/mol×K	589.48	Joback Method
cpg	537.95	J/mol×K	727.16	Joback Method
dvisc	0.0000795	Pa×s	561.94	Joback Method
dvisc	0.0001402	Pa×s	510.63	Joback Method

dvisc	0.0002805	Pa×s	459.31	Joback Method
dvisc	0.0006684	Pa×s	408.00	Joback Method
dvisc	0.0020442	Pa×s	356.69	Joback Method
dvisc	0.0091029	Pa×s	305.37	Joback Method
dvisc	0.0741066	Pa×s	254.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R412687&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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