2-Octen-4-ol, 2-methyl-

Inchi: InChI=1S/C9H18O/c1-4-5-6-9(10)7-8(2)3/h7,9-10H,4-6H2,1-3H3
InchiKey: PNLIZTGZMGUPNP-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CCCCC(O)C=C(C)C
Mol. weight [g/mol]: 142.24
CAS: 65885-49-6

Physical Properties

Property code	Value	Unit	Source
gf	-42.69	kJ/mol	Joback Method
hf	-279.17	kJ/mol	Joback Method
hfus	18.52	kJ/mol	Joback Method
hvap	51.96	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.504		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
tb	501.10	K	Joback Method
tc	672.83	K	Joback Method
tf	217.97	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.19	J/mol×K	501.10	Joback Method
cpg	329.73	J/mol×K	529.72	Joback Method
cpg	341.72	J/mol×K	558.34	Joback Method
cpg	353.17	J/mol×K	586.96	Joback Method
cpg	364.10	J/mol×K	615.58	Joback Method
cpg	374.54	J/mol×K	644.21	Joback Method
cpg	384.52	J/mol×K	672.83	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=C65885496&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