2,3-Dimethyl-4-penten-2-ol

Inchi: InChI=1S/C7H14O/c1-5-6(2)7(3,4)8/h5,8H,1-4H3/b6-5+
InchiKey: PGCNLWGJQKSWAP-AATRIKPKSA-N
Formula: C7H14O
SMILES: CC=C(C)C(C)(C)O
Mol. weight [g/mol]: 114.19
CAS: 19781-52-3

Physical Properties

Property code	Value	Unit	Source
gf	-54.25	kJ/mol	Joback Method
hf	-241.36	kJ/mol	Joback Method
hfus	9.45	kJ/mol	Joback Method
hvap	46.60	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.723		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
tb	452.55	K	Joback Method
tc	633.86	K	Joback Method
tf	212.85	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.15	J/mol×K	452.55	Joback Method
cpg	245.58	J/mol×K	482.77	Joback Method
cpg	256.37	J/mol×K	512.99	Joback Method
cpg	266.55	J/mol×K	543.21	Joback Method
cpg	276.16	J/mol×K	573.42	Joback Method
cpg	285.22	J/mol×K	603.64	Joback Method
cpg	293.78	J/mol×K	633.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19781523&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume