4-Penten-1-ol, 2,2,4-trimethyl-

Inchi: InChI=1S/C8H16O/c1-7(2)5-8(3,4)6-9/h9H,1,5-6H2,2-4H3
InchiKey: IPCBOHBHGXVTER-UHFFFAOYSA-N
Formula: C8H16O
SMILES: C=C(C)CC(C)(C)CO
Mol. weight [g/mol]: 128.21
CAS: 53907-70-3

Physical Properties

Property code	Value	Unit	Source
gf	-38.21	kJ/mol	Joback Method
hf	-253.79	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	48.20	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.971		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
ripol	1592.00		NIST Webbook
tb	467.95	K	Joback Method
tc	643.10	K	Joback Method
tf	227.44	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.64	J/mol×K	467.95	Joback Method
cpg	287.79	J/mol×K	497.14	Joback Method
cpg	299.32	J/mol×K	526.33	Joback Method
cpg	310.26	J/mol×K	555.53	Joback Method
cpg	320.64	J/mol×K	584.72	Joback Method
cpg	330.48	J/mol×K	613.91	Joback Method
cpg	339.82	J/mol×K	643.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53907703&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume