(1S,2R,4S,7R)-7-((E)-5-Hydroxy-4-methylpent-3-en

Inchi: InChI=1S/C15H26O2/c1-11(10-16)5-4-7-14(2)12-6-8-15(14,3)13(17)9-12/h5,12-13,16-17
InchiKey: FUCSWNUANQRDFQ-VZUCSPMQSA-N
Formula: C15H26O2
SMILES: CC(=CCCC1(C)C2CCC1(C)C(O)C2)CO
Mol. weight [g/mol]: 238.37
CAS: 201731-87-5

Physical Properties

Property code	Value	Unit	Source
gf	-43.55	kJ/mol	Joback Method
hf	-420.72	kJ/mol	Joback Method
hfus	25.39	kJ/mol	Joback Method
hvap	79.46	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	2.892		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1958.80		NIST Webbook
rinpol	1958.80		NIST Webbook
tb	739.89	K	Joback Method
tc	930.76	K	Joback Method
tf	433.09	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.68	J/mol×K	739.89	Joback Method
cpg	669.60	J/mol×K	771.70	Joback Method
cpg	685.33	J/mol×K	803.51	Joback Method
cpg	701.02	J/mol×K	835.32	Joback Method
cpg	716.88	J/mol×K	867.14	Joback Method
cpg	733.09	J/mol×K	898.95	Joback Method
cpg	749.81	J/mol×K	930.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C201731875&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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