7-(2-Hydroxypropan-2-yl)-1,4a-dimethyldecahydro

Inchi: InChI=1S/C15H28O2/c1-13(2,16)11-6-9-14(3)7-5-8-15(4,17)12(14)10-11/h11-12,16-17H
InchiKey: LKKDASYGWYYFIK-UHFFFAOYSA-N
Formula: C15H28O2
SMILES: CC(C)(O)C1CCC2(C)CCCC(C)(O)C2C1
Mol. weight [g/mol]: 240.38
CAS: 92857-25-5

Physical Properties

Property code	Value	Unit	Source
gf	-148.68	kJ/mol	Joback Method
hf	-555.38	kJ/mol	Joback Method
hfus	12.78	kJ/mol	Joback Method
hvap	78.64	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.115		Crippen Method
mcvol	212.230	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	1782.00		NIST Webbook
rinpol	1782.00		NIST Webbook
tb	745.43	K	Joback Method
tc	949.62	K	Joback Method
tf	443.99	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.98	J/mol×K	745.43	Joback Method
cpg	708.38	J/mol×K	779.46	Joback Method
cpg	726.35	J/mol×K	813.49	Joback Method
cpg	744.12	J/mol×K	847.52	Joback Method
cpg	761.87	J/mol×K	881.55	Joback Method
cpg	779.83	J/mol×K	915.59	Joback Method
cpg	798.19	J/mol×K	949.62	Joback Method

Sources

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=C92857255&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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