(3aRS,4SR,7aSR)-(Octahydro-1H-inden-4-yl) methanol

Inchi: InChI=1S/C10H18O/c11-7-9-5-1-3-8-4-2-6-10(8)9/h8-11H,1-7H2
InchiKey: JAZXFQSTFJATMJ-UHFFFAOYSA-N
Formula: C10H18O
SMILES: OCC1CCCC2CCCC12
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-26.01	kJ/mol	Joback Method
hf	-295.18	kJ/mol	Joback Method
hfus	16.79	kJ/mol	Joback Method
hvap	54.57	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.195		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	1310.00		NIST Webbook
rinpol	1310.00		NIST Webbook
ripol	1989.00		NIST Webbook
ripol	1989.00		NIST Webbook
tb	542.00	K	Joback Method
tc	741.43	K	Joback Method
tf	284.36	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.79	J/mol×K	542.00	Joback Method
cpg	373.42	J/mol×K	575.24	Joback Method
cpg	390.04	J/mol×K	608.48	Joback Method
cpg	405.70	J/mol×K	641.72	Joback Method
cpg	420.44	J/mol×K	674.96	Joback Method
cpg	434.31	J/mol×K	708.20	Joback Method

cpg	447.36	J/mol×K	741.43	Joback Method
dvisc	0.0142324	Pa×s	284.36	Joback Method
dvisc	0.0048522	Pa×s	327.30	Joback Method
dvisc	0.0021233	Pa×s	370.24	Joback Method
dvisc	0.0011033	Pa×s	413.18	Joback Method
dvisc	0.0006485	Pa×s	456.12	Joback Method
dvisc	0.0004176	Pa×s	499.06	Joback Method
dvisc	0.0002884	Pa×s	542.00	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R586699&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
dvisc: Dynamic viscosity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume