4a(2H)-Naphthalenol, octahydro-4,8a-dimethyl-,(4«alpha»,4a«alpha»,8a«

Other names: 4a(2H)-Naphthalenol, octahydro-4,8a-dimethyl-, [4S-(4«alpha»,4a«alpha»,8a«beta»)]-Geosmin

4a-«alpha»-(2H)-Naphthol, octahydro-4-«alpha»,8a-«beta»-dimethyl-

[4S-(4«alpha»,4a«alpha»,8a«beta»)]-octahydro-4,8a-dimethyl-4a(2H)-naphthol

Inchi: InChI=1S/C12H22O/c1-10-6-5-8-11(2)7-3-4-9-12(10,11)13/h10,13H,3-9H2,1-2H3/t10-,11

InchiKey: JLPUXFOGCDVKGO-GRYCIOLGSA-N

Formula: C12H22O

SMILES: CC1CCCC2(C)CCCCC12O

Mol. weight [g/mol]: 182.30

CAS: 19700-21-1

Physical Properties

Property code	Value	Unit	Source
gf	-32.25	kJ/mol	Joback Method
hf	-312.14	kJ/mol	Joback Method
hfus	7.27	kJ/mol	Joback Method
hvap	56.89	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.118		Crippen Method
mcvol	164.090	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1444.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1430.00		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1858.00		NIST Webbook
ripol	1810.00		NIST Webbook
ripol	1823.00		NIST Webbook
ripol	1808.00		NIST Webbook

ripol	1821.00		NIST Webbook
tb	592.51	K	Joback Method
tc	808.40	K	Joback Method
tf	351.18	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.91	J/mol×K	592.51	Joback Method
cpg	474.02	J/mol×K	628.49	Joback Method
cpg	491.99	J/mol×K	664.47	Joback Method
cpg	509.04	J/mol×K	700.46	Joback Method
cpg	525.40	J/mol×K	736.44	Joback Method
cpg	541.29	J/mol×K	772.42	Joback Method
cpg	556.93	J/mol×K	808.40	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19700211&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
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