2-((2S,4aR)-4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahyd

Other names: 2-Naphthalenemethanol, 1,2,3,4,4a,5,6,7-octahydro-«alpha»,«alpha»,4a,8-tetramethyl-, (2S,4aR)-
epi-«gamma»-Eudesmol
7-epi-«gamma»-Eudesmol

Inchi: InChI=1S/C15H26O/c1-11-6-5-8-15(4)9-7-12(10-13(11)15)14(2,3)16/h12,16H,5-10H2,1-4

InchiKey: WMOPMQRJLLIEJV-UHFFFAOYSA-N

Formula: C15H26O

SMILES: CC1=C2CC(C(C)(C)O)CCC2(C)CCC1

Mol. weight [g/mol]: 222.37

CAS: 117066-77-0

Physical Properties

Property code	Value	Unit	Source
gf	19.75	kJ/mol	Joback Method
hf	-342.87	kJ/mol	Joback Method
hfus	13.30	kJ/mol	Joback Method
hvap	65.35	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.064		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1664.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1664.00		NIST Webbook
tb	671.47	K	Joback Method
tc	884.60	K	Joback Method
tf	393.55	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.14	J/mol×K	671.47	Joback Method
cpg	615.41	J/mol×K	706.99	Joback Method
cpg	633.66	J/mol×K	742.51	Joback Method

cpg	651.05	J/mol×K	778.04	Joback Method
cpg	667.73	J/mol×K	813.56	Joback Method
cpg	683.86	J/mol×K	849.08	Joback Method
cpg	699.60	J/mol×K	884.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C117066770&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume