(4R,4aR)-4,4a-Dimethyl-6-(prop-1-en-2-yl)-1,2,3,4,4

Inchi: InChI=1S/C15H22/c1-11(2)13-8-9-14-7-5-6-12(3)15(14,4)10-13/h9-10,12H,1,5-8H2,2-4H
InchiKey: WHNNPKNATREGBK-SWLSCSKDSA-N
Formula: C15H22
SMILES: C=C(C)C1=CC2(C)C(=CC1)CCCC2C
Mol. weight [g/mol]: 202.34
CAS: 28908-26-1

Physical Properties

Property code	Value	Unit	Source
gf	262.98	kJ/mol	Joback Method
hf	-8.47	kJ/mol	Joback Method
hfus	15.25	kJ/mol	Joback Method
hvap	49.67	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.645		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1540.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1536.90		NIST Webbook
tb	578.24	K	Joback Method
tc	806.39	K	Joback Method
tf	315.35	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.59	J/mol×K	578.24	Joback Method
cpg	501.10	J/mol×K	616.26	Joback Method
cpg	521.21	J/mol×K	654.29	Joback Method
cpg	540.12	J/mol×K	692.31	Joback Method
cpg	557.97	J/mol×K	730.34	Joback Method

cpg	574.96	J/mol×K	768.36	Joback Method
cpg	591.25	J/mol×K	806.39	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28908261&Units=SI

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

Latest version available from:
https://www.chemeo.com/cid/74-960-4/4R-4aR-4-4a-Dimethyl-6-prop-1-en-2-yl-1-2-3-4-4a-7-hexahydronaphthalene.
Generated by Cheméo on 2024-04-27 05:54:54.371166375 +0000 UTC m=+16486543.291743708.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.