

(2R,3R,6S)-6-Isopropyl-3-methyl-2-(prop-1-en-2-yl)

Inchi:	InChI=1S/C15H24O/c1-7-15(6)9-8-12(10(2)3)14(16)13(15)11(4)5/h7,10,12-13H,1,4,8-9H
InchiKey:	GWHRSRIPLDHJHR-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	<chem>C=CC1(C)CCC(C(C)C)C(=O)C1C(=C)C</chem>
Mol. weight [g/mol]:	220.35
CAS:	39020-72-9

Physical Properties

Property code	Value	Unit	Source
gf	121.06	kJ/mol	Joback Method
hf	-225.96	kJ/mol	Joback Method
hfus	14.40	kJ/mol	Joback Method
hvap	50.24	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	4.006		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
rinpol	1497.70		NIST Webbook
rinpol	1497.70		NIST Webbook
tb	613.67	K	Joback Method
tc	834.59	K	Joback Method
tf	317.35	K	Joback Method
vc	0.768	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.57	J/molxK	613.67	Joback Method
cpg	574.78	J/molxK	650.49	Joback Method
cpg	595.82	J/molxK	687.31	Joback Method
cpg	615.78	J/molxK	724.13	Joback Method
cpg	634.76	J/molxK	760.95	Joback Method
cpg	652.87	J/molxK	797.77	Joback Method
cpg	670.21	J/molxK	834.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39020729&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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