

Cedrane

Other names:	8«beta»H-Cedrane 8«alpha»H-Cedrane epi-cedrane «beta»-Cedrane «alpha»-cedrane
Inchi:	InChI=1S/C15H26/c1-10-7-8-15-9-12(10)14(3,4)13(15)6-5-11(15)2/h10-13H,5-9H2,1-4H3
InchiKey:	JJTQQGNEXQKQRF-RCVBVVPMSA-N
Formula:	C15H26
SMILES:	CC1CCC23CC1C(C)(C)C2CCC3C
Mol. weight [g/mol]:	206.37
CAS:	13567-55-0

Physical Properties

Property code	Value	Unit	Source
gf	199.36	kJ/mol	Joback Method
hf	-177.39	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	45.84	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.495		Crippen Method
mcvol	189.630	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1455.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1479.00		NIST Webbook

ripol	1458.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1470.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1627.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1662.00		NIST Webbook
ripol	1633.00		NIST Webbook
ripol	1633.00		NIST Webbook
tb	557.83	K	Joback Method
tc	780.06	K	Joback Method
tf	340.67	K	Joback Method
vc	0.724	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.52	J/mol×K	557.83	Joback Method
cpg	547.59	J/mol×K	594.87	Joback Method
cpg	570.94	J/mol×K	631.91	Joback Method
cpg	592.86	J/mol×K	668.95	Joback Method
cpg	613.64	J/mol×K	705.99	Joback Method
cpg	633.54	J/mol×K	743.02	Joback Method
cpg	652.86	J/mol×K	780.06	Joback Method

Sources

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=C13567550&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
ri_{npol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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