

(-)-Aristolene

Other names:	Aristolene Aristolen
Inchi:	InChI=1S/C15H24/c1-10-6-5-7-11-8-9-12-13(14(12,2)3)15(10,11)4/h8,10,12-13H,5-7,9H
InchiKey:	FOB XOZMHEKILEY-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC1CCCC2=CCC3C(C3(C)C)C21C
Mol. weight [g/mol]:	204.35
CAS:	6831-16-9

Physical Properties

Property code	Value	Unit	Source
gf	227.40	kJ/mol	Joback Method
hf	-110.74	kJ/mol	Joback Method
hfus	15.19	kJ/mol	Joback Method
hvap	47.10	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1418.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1428.30		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1428.30		NIST Webbook
rinpol	1417.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1552.00		NIST Webbook

ripol	1574.00		NIST Webbook
ripol	1553.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1589.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1572.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1553.00		NIST Webbook
tb	566.64	K	Joback Method
tc	792.17	K	Joback Method
tf	358.19	K	Joback Method
vc	0.711	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.55	J/mol×K	566.64	Joback Method
cpg	526.55	J/mol×K	604.23	Joback Method
cpg	547.97	J/mol×K	641.82	Joback Method
cpg	568.10	J/mol×K	679.41	Joback Method
cpg	587.25	J/mol×K	716.99	Joback Method
cpg	605.70	J/mol×K	754.58	Joback Method
cpg	623.74	J/mol×K	792.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6831169&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
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
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

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