

Amorphane-a (isocadinane)

Inchi:	InChI=1S/C15H28/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h10-15H,5-9H2,1-4H3/t1
InchiKey:	FZZNNPQZDRVKLU-QXRZNBQRSA-N
Formula:	C15H28
SMILES:	CC1CCC2C(C)CCC(C(C)C)C2C1
Mol. weight [g/mol]:	208.38

Physical Properties

Property code	Value	Unit	Source
gf	122.95	kJ/mol	Joback Method
hf	-298.27	kJ/mol	Joback Method
hfus	22.17	kJ/mol	Joback Method
hvap	48.18	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.741		Crippen Method
mcvol	200.490	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinsol	1455.00		NIST Webbook
tb	558.71	K	Joback Method
tc	767.90	K	Joback Method
tf	252.89	K	Joback Method
vc	0.749	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.96	J/molxK	558.71	Joback Method
cpg	567.48	J/molxK	593.57	Joback Method
cpg	592.55	J/molxK	628.44	Joback Method
cpg	616.21	J/molxK	663.30	Joback Method
cpg	638.49	J/molxK	698.17	Joback Method
cpg	659.45	J/molxK	733.03	Joback Method
cpg	679.13	J/molxK	767.90	Joback Method
dvisc	0.0025609	Paxs	252.89	Joback Method
dvisc	0.0014675	Paxs	303.86	Joback Method

dvisc	0.0009869	Paxs	354.83	Joback Method
dvisc	0.0007332	Paxs	405.80	Joback Method
dvisc	0.0005821	Paxs	456.77	Joback Method
dvisc	0.0004840	Paxs	507.74	Joback Method
dvisc	0.0004163	Paxs	558.71	Joback Method

Sources

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=R306611&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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