

Acepleiadane

Inchi:	InChI=1S/C16H16/c1-2-4-12-6-8-14-10-9-13-7-5-11(3-1)15(12)16(13)14/h5-8H,1-4,9-10H
InchiKey:	MODFRFVMVVZBAZ-UHFFFAOYSA-N
Formula:	C16H16
SMILES:	<chem>c1cc2c3c(ccc4c3c1CCCC4)CC2</chem>
Mol. weight [g/mol]:	208.30
CAS:	518-02-5

Physical Properties

Property code	Value	Unit	Source
gf	401.30	kJ/mol	Joback Method
hf	194.43	kJ/mol	Joback Method
hfus	20.83	kJ/mol	Joback Method
hvap	58.22	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	3.817		Crippen Method
mcvol	171.360	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	653.88	K	Joback Method
tc	902.59	K	Joback Method
tf	423.64	K	Joback Method
vc	0.661	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.14	J/molxK	653.88	Joback Method
cpg	472.13	J/molxK	695.33	Joback Method
cpg	487.82	J/molxK	736.78	Joback Method
cpg	502.41	J/molxK	778.23	Joback Method
cpg	516.07	J/molxK	819.68	Joback Method
cpg	529.01	J/molxK	861.14	Joback Method
cpg	541.40	J/molxK	902.59	Joback Method
dvisc	0.0023079	Paxs	423.64	Joback Method
dvisc	0.0019684	Paxs	462.01	Joback Method

dvisc	0.0017204	Paxs	500.39	Joback Method
dvisc	0.0015327	Paxs	538.76	Joback Method
dvisc	0.0013866	Paxs	577.13	Joback Method
dvisc	0.0012702	Paxs	615.51	Joback Method
dvisc	0.0011757	Paxs	653.88	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=C518025&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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