

Bicyclooctyl-3,3'-diene

Inchi:	InChI=1S/C16H26/c1-3-7-11-15(12-8-4-1)16-13-9-5-2-6-10-14-16/h3,5,7,9,15-16H,1-2,4,
InchiKey:	SNIUWVJGQPWRBT-DLYLGUBQSA-N
Formula:	C16H26
SMILES:	C1=CCC(C2CC=CCCCC2)CCCC1
Mol. weight [g/mol]:	218.38

Physical Properties

Property code	Value	Unit	Source
gf	144.26	kJ/mol	Joback Method
hf	-174.01	kJ/mol	Joback Method
hfus	14.91	kJ/mol	Joback Method
hvap	53.34	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	5.259		Crippen Method
mcvol	205.980	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinsol	1737.00		NIST Webbook
tb	619.98	K	Joback Method
tc	872.00	K	Joback Method
tf	272.28	K	Joback Method
vc	0.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.31	J/molxK	619.98	Joback Method
cpg	598.82	J/molxK	661.98	Joback Method
cpg	626.13	J/molxK	703.99	Joback Method
cpg	651.28	J/molxK	745.99	Joback Method
cpg	674.30	J/molxK	787.99	Joback Method
cpg	695.24	J/molxK	830.00	Joback Method
cpg	714.12	J/molxK	872.00	Joback Method
dvisc	0.0168318	Paxs	272.28	Joback Method
dvisc	0.0029020	Paxs	330.23	Joback Method

dvisc	0.0008457	Paxs	388.18	Joback Method
dvisc	0.0003395	Paxs	446.13	Joback Method
dvisc	0.0001681	Paxs	504.08	Joback Method
dvisc	0.0000962	Paxs	562.03	Joback Method
dvisc	0.0000611	Paxs	619.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136497&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
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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