

trans,trans,cis-Bicyclo[4.4.0]decane, 2,4-dimethyl

Inchi: InChI=1S/C12H22/c1-9-7-10(2)12-6-4-3-5-11(12)8-9/h9-12H,3-8H2,1-2H3/t9-,10-,11-,12-
InchiKey: GOSLMGVBJBCFKP-XOGOEWOHSA-N
Formula: C12H22
SMILES: CC1CC(C)C2CCCCC2C1
Mol. weight [g/mol]: 166.30

Physical Properties

Property code	Value	Unit	Source
gf	107.84	kJ/mol	Joback Method
hf	-210.73	kJ/mol	Joback Method
hfus	16.85	kJ/mol	Joback Method
hvap	42.20	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.859		Crippen Method
mcvol	158.220	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	1230.00		NIST Webbook
rinpol	1230.00		NIST Webbook
ripol	1354.00		NIST Webbook
tb	495.18	K	Joback Method
tc	710.00	K	Joback Method
tf	238.32	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.66	J/molxK	495.18	Joback Method
cpg	407.11	J/molxK	530.98	Joback Method
cpg	430.21	J/molxK	566.79	Joback Method
cpg	451.99	J/molxK	602.59	Joback Method
cpg	472.51	J/molxK	638.39	Joback Method
cpg	491.81	J/molxK	674.20	Joback Method
cpg	509.92	J/molxK	710.00	Joback Method

dvisc	0.0022593	Paxs	238.32	Joback Method
dvisc	0.0013842	Paxs	281.13	Joback Method
dvisc	0.0009653	Paxs	323.94	Joback Method
dvisc	0.0007322	Paxs	366.75	Joback Method
dvisc	0.0005885	Paxs	409.56	Joback Method
dvisc	0.0004929	Paxs	452.37	Joback Method
dvisc	0.0004257	Paxs	495.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R531565&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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