trans,trans,trans-Bicyclo[4.4.0]decane, 2,3-dimethyl

Inchi: InChI=1S/C12H22/c1-9-7-8-11-5-3-4-6-12(11)10(9)2/h9-12H,3-8H2,1-2H3/t9-,10-,11-,12

InchiKey: FHEIPFHZECVFRS-XOGOEWOHSA-N

Formula: C12H22

SMILES: CC1CCC2CCCCC2C1C

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	1246.00		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1379.00		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/mol×K	495.18	Joback Method
cpg	407.11	J/mol×K	530.98	Joback Method
cpg	430.21	J/mol×K	566.79	Joback Method
cpg	451.99	J/mol×K	602.59	Joback Method
cpg	472.51	J/mol×K	638.39	Joback Method
cpg	491.81	J/mol×K	674.20	Joback Method
cpg	509.92	J/mol×K	710.00	Joback Method

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R531649&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
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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