

trans,cis-Bicyclo[4.4.0]decane, 3-ethyl

Inchi:	InChI=1S/C12H22/c1-2-10-7-8-11-5-3-4-6-12(11)9-10/h10-12H,2-9H2,1H3/t10-,11+,12?/
InchiKey:	HLQZZLGOHWUHQM-UBNQQGINQSA-N
Formula:	C12H22
SMILES:	CCC1CCC2CCCCC2C1
Mol. weight [g/mol]:	166.30

Physical Properties

Property code	Value	Unit	Source
gf	115.55	kJ/mol	Joback Method
hf	-190.39	kJ/mol	Joback Method
hfus	15.78	kJ/mol	Joback Method
hvap	42.51	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	4.003		Crippen Method
mcvol	158.220	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinsol	1274.00		NIST Webbook
ripol	1414.00		NIST Webbook
tb	499.85	K	Joback Method
tc	714.86	K	Joback Method
tf	242.56	K	Joback Method
vc	0.589	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.91	J/molxK	499.85	Joback Method
cpg	406.90	J/molxK	535.69	Joback Method
cpg	429.53	J/molxK	571.52	Joback Method
cpg	450.82	J/molxK	607.36	Joback Method
cpg	470.85	J/molxK	643.19	Joback Method
cpg	489.65	J/molxK	679.03	Joback Method
cpg	507.27	J/molxK	714.86	Joback Method
dvisc	0.0034936	Paxs	242.56	Joback Method

dvisc	0.0018638	Paxs	285.44	Joback Method
dvisc	0.0011717	Paxs	328.32	Joback Method
dvisc	0.0008200	Paxs	371.20	Joback Method
dvisc	0.0006179	Paxs	414.09	Joback Method
dvisc	0.0004910	Paxs	456.97	Joback Method
dvisc	0.0004058	Paxs	499.85	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=R531352&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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