cis,trans-Bicyclo[4.4.0]decane, 2-ethyl

Inchi: InChI=1S/C12H22/c1-2-10-7-5-8-11-6-3-4-9-12(10)11/h10-12H,2-9H2,1H3/t10-,11-,12+/r

InchiKey: HUMCBDCARGDFNV-UTUOFQBUSA-N

Formula: C12H22

SMILES: CCC1CCCC2CCCCC12

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
rinpol	1270.00		NIST Webbook
rinpol	1270.00		NIST Webbook
ripol	1377.00		NIST Webbook
tb	499.85	K	Joback Method
tc	714.86	K	Joback Method
tf	242.56	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0034936	Pa×s	242.56	Joback Method
dvisc	0.0018638	Pa×s	285.44	Joback Method
dvisc	0.0011717	Pa×s	328.32	Joback Method
dvisc	0.0008200	Pa×s	371.20	Joback Method
dvisc	0.0006179	Pa×s	414.09	Joback Method
dvisc	0.0004910	Pa×s	456.97	Joback Method
dvisc	0.0004058	Pa×s	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=R531134&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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