

(trans-1,2-methylene)butyl-cyclopropane

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C8H14/c1-2-6-5-8(6)7-3-4-7/h6-8H,2-5H2,1H3/t6-,8+/m1/s1

VDKZAQZRSgyRSL-SVRRBLITSA-N

C8H14

CCC1CC1C1CC1

110.20

Physical Properties

Property code	Value	Unit	Source
gf	130.27	kJ/mol	Joback Method
hf	-83.19	kJ/mol	Joback Method
hfus	13.82	kJ/mol	Joback Method
hvap	32.92	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.442		Crippen Method
mcvol	101.860	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	790.40		NIST Webbook
rinpol	792.70		NIST Webbook
rinpol	794.70		NIST Webbook
rinpol	794.70		NIST Webbook
tb	391.25	K	Joback Method
tc	583.79	K	Joback Method
tf	211.56	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.95	J/mol×K	391.25	Joback Method
cpg	274.67	J/mol×K	551.70	Joback Method
cpg	261.67	J/mol×K	519.61	Joback Method
cpg	247.85	J/mol×K	487.52	Joback Method
cpg	233.16	J/mol×K	455.43	Joback Method
cpg	217.54	J/mol×K	423.34	Joback Method

cpg	286.89	J/mol×K	583.79	Joback Method
dvisc	0.0004955	Pa×s	391.25	Joback Method
dvisc	0.0004734	Pa×s	361.30	Joback Method
dvisc	0.0004485	Pa×s	331.35	Joback Method
dvisc	0.0004204	Pa×s	301.40	Joback Method
dvisc	0.0003885	Pa×s	271.46	Joback Method
dvisc	0.0003521	Pa×s	241.51	Joback Method
dvisc	0.0003103	Pa×s	211.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R138002&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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