

(trans-4,5-Methylene)octyl-cyclopropane

Inchi:	InChI=1S/C12H22/c1-2-4-11-9-12(11)6-3-5-10-7-8-10/h10-12H,2-9H2,1H3/t11-,12-/m1/s
InchiKey:	CVXDKCAUIWVFCZ-VXGBXAGGSA-N
Formula:	C12H22
SMILES:	CCCC1CC1CCCC1CC1
Mol. weight [g/mol]:	166.30

Physical Properties

Property code	Value	Unit	Source
gf	163.95	kJ/mol	Joback Method
hf	-165.75	kJ/mol	Joback Method
hfus	24.18	kJ/mol	Joback Method
hvap	41.82	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	4.003		Crippen Method
mcvol	158.220	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1171.20		NIST Webbook
rinpol	1168.10		NIST Webbook
tb	482.77	K	Joback Method
tc	668.31	K	Joback Method
tf	256.64	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.19	J/mol×K	482.77	Joback Method
cpg	399.79	J/mol×K	513.69	Joback Method
cpg	418.34	J/mol×K	544.62	Joback Method
cpg	435.89	J/mol×K	575.54	Joback Method
cpg	452.50	J/mol×K	606.46	Joback Method
cpg	468.22	J/mol×K	637.39	Joback Method
cpg	483.10	J/mol×K	668.31	Joback Method
dvisc	0.0010963	Pa×s	256.64	Joback Method

dvisc	0.0010116	Pa×s	294.33	Joback Method
dvisc	0.0009507	Pa×s	332.02	Joback Method
dvisc	0.0009049	Pa×s	369.70	Joback Method
dvisc	0.0008692	Pa×s	407.39	Joback Method
dvisc	0.0008406	Pa×s	445.08	Joback Method
dvisc	0.0008172	Pa×s	482.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R138166&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

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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