

(trans-2,3-Methylene)octyl-cyclopropane

Inchi:	InChI=1S/C12H22/c1-2-3-4-5-11-9-12(11)8-10-6-7-10/h10-12H,2-9H2,1H3/t11-,12-/m0/s
InchiKey:	GPKLFCSLPFSMLG-RYUDHWPXSA-N
Formula:	C12H22
SMILES:	CCCCC1CC1CC1CC1
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	1166.80		NIST Webbook
rinpol	1166.80		NIST Webbook
rinpol	1170.10		NIST Webbook
tb	482.77	K	Joback Method
tc	668.31	K	Joback Method
tf	256.64	K	Joback Method
vc	0.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.19	J/molxK	482.77	Joback Method
cpg	399.79	J/molxK	513.69	Joback Method
cpg	418.34	J/molxK	544.62	Joback Method
cpg	435.89	J/molxK	575.54	Joback Method
cpg	452.50	J/molxK	606.46	Joback Method
cpg	468.22	J/molxK	637.39	Joback Method
cpg	483.10	J/molxK	668.31	Joback Method

dvisc	0.0010963	Paxs	256.64	Joback Method
dvisc	0.0010116	Paxs	294.33	Joback Method
dvisc	0.0009507	Paxs	332.02	Joback Method
dvisc	0.0009049	Paxs	369.70	Joback Method
dvisc	0.0008692	Paxs	407.39	Joback Method
dvisc	0.0008406	Paxs	445.08	Joback Method
dvisc	0.0008172	Paxs	482.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R138097&Units=SI

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
mvol:	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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