

VINYLIDENE-CYCLOHEXANE

Inchi:	InChI=1S/C8H12/c1-2-8-6-4-3-5-7-8/h1,3-7H2
InchiKey:	HZHTYEIEGPBKKS-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	C=C=C1CCCCC1
Mol. weight [g/mol]:	108.18

Physical Properties

Property code	Value	Unit	Source
hfus	8.21	kJ/mol	Joback Method
ie	8.69	eV	NIST Webbook
logp	2.662		Crippen Method
mcvol	104.120	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.09	J/mol×K	409.09	Joback Method
cpg	204.73	J/mol×K	445.27	Joback Method
cpg	218.69	J/mol×K	481.44	Joback Method
cpg	231.98	J/mol×K	517.62	Joback Method
cpg	244.61	J/mol×K	553.79	Joback Method
cpg	256.59	J/mol×K	589.97	Joback Method
cpg	267.93	J/mol×K	626.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5664200&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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