

# (7R, 8S)-cis-7,8-epoxy-2-methyloctadecane [(+)-disparlure]

Inchi:	InChI=1S/C19H38O/c1-4-5-6-7-8-9-10-11-15-18-19(20-18)16-13-12-14-17(2)3/h17-19H,4
InchiKey:	HFOFYNMWYRXIBP-OALUTQOASA-N
Formula:	C19H38O
SMILES:	CCCCCCCCC1OC1CCCC(C)C
Mol. weight [g/mol]:	282.50

## Physical Properties

Property code	Value	Unit	Source
gf	73.58	kJ/mol	Joback Method
hf	-520.31	kJ/mol	Joback Method
hfus	48.63	kJ/mol	Joback Method
hvap	61.61	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	6.501		Crippen Method
mcvol	273.580	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinpol	2032.00		NIST Webbook
tb	662.70	K	Joback Method
tc	832.43	K	Joback Method
tf	329.16	K	Joback Method
vc	1.071	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.45	J/molxK	662.70	Joback Method
cpg	830.42	J/molxK	690.99	Joback Method
cpg	850.44	J/molxK	719.28	Joback Method
cpg	869.55	J/molxK	747.57	Joback Method
cpg	887.80	J/molxK	775.86	Joback Method
cpg	905.21	J/molxK	804.15	Joback Method
cpg	921.83	J/molxK	832.43	Joback Method
dvisc	0.0033344	Paxs	329.16	Joback Method
dvisc	0.0016515	Paxs	384.75	Joback Method

dvisc	0.0009768	Paxs	440.34	Joback Method
dvisc	0.0006499	Paxs	495.93	Joback Method
dvisc	0.0004694	Paxs	551.52	Joback Method
dvisc	0.0003599	Paxs	607.11	Joback Method
dvisc	0.0002885	Paxs	662.70	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R501618&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R501618&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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