Disparlure

Other names:	Oxirane, 2-decyl-3-(5-methylhexyl)-, cis- (.+/-cis-7,8-Epoxy-2-methyloctadecane 2-Decyl-3-(5-methylhexyl)oxirane, (Z)- cis-7,8-Epoxy-2-methyloctadecane Epoxan (Z)-7,8-Epoxy-2-methyloctadecane Atralymon (+/-)-cis-Disparlure Oxirane, 2-decyl-3-(5-methylhexyl)-, (2R,3S)-rel-
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-RBUKOAKNSA-N
Formula:	C19H38O
SMILES:	CCCCCCCCCCC1OC1CCCCC(C)C
Mol. weight [g/mol]:	282.50
CAS:	29804-22-6

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
rinpol	2032.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	2028.00		NIST Webbook
rinpol	1990.00		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/mol×K	662.70	Joback Method
cpg	905.21	J/mol×K	804.15	Joback Method
cpg	887.80	J/mol×K	775.86	Joback Method
cpg	869.55	J/mol×K	747.57	Joback Method
cpg	850.44	J/mol×K	719.28	Joback Method
cpg	830.42	J/mol×K	690.99	Joback Method
cpg	921.83	J/mol×K	832.43	Joback Method
dvisc	0.0002885	Pa×s	662.70	Joback Method
dvisc	0.0003599	Pa×s	607.11	Joback Method
dvisc	0.0004694	Pa×s	551.52	Joback Method
dvisc	0.0006499	Pa×s	495.93	Joback Method
dvisc	0.0009768	Pa×s	440.34	Joback Method
dvisc	0.0016515	Pa×s	384.75	Joback Method
dvisc	0.0033344	Pa×s	329.16	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29804226&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