

1,E-11,Z-13-Octadecatriene

Inchi:	InChI=1S/C18H32/c1-3-5-7-9-11-13-15-17-18-16-14-12-10-8-6-4-2/h3,10,12,14,16H,1,4-
InchiKey:	XWCKCHRCDXCUHK-OMGSKEOWSA-N
Formula:	C18H32
SMILES:	C=CCCCCCCCC=CC=CCCC
Mol. weight [g/mol]:	248.45
CAS:	80625-36-1

Physical Properties

Property code	Value	Unit	Source
gf	348.96	kJ/mol	Joback Method
hf	-54.98	kJ/mol	Joback Method
hfus	41.50	kJ/mol	Joback Method
hvap	54.91	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.596		Crippen Method
mcvol	251.580	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	1685.00		NIST Webbook
tb	616.24	K	Joback Method
tc	787.33	K	Joback Method
tf	280.70	K	Joback Method
vc	0.985	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.23	J/molxK	616.24	Joback Method
cpg	748.73	J/molxK	758.82	Joback Method
cpg	733.00	J/molxK	730.30	Joback Method
cpg	716.53	J/molxK	701.79	Joback Method
cpg	699.27	J/molxK	673.27	Joback Method
cpg	681.18	J/molxK	644.76	Joback Method
cpg	763.77	J/molxK	787.33	Joback Method
dvisc	0.0000940	Paxs	616.24	Joback Method

dvisc	0.0001277	Paxs	560.32	Joback Method
dvisc	0.0001857	Paxs	504.39	Joback Method
dvisc	0.0002965	Paxs	448.47	Joback Method
dvisc	0.0005409	Paxs	392.55	Joback Method
dvisc	0.0012050	Paxs	336.62	Joback Method
dvisc	0.0036935	Paxs	280.70	Joback Method

Sources

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=C80625361&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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