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/C=C/C=C\CCCC
Mol. weight [g/mol]: 248.45

Physical Properties

Property code	Value	Unit	Source
af	0.6309		Cheméo Relay (1.0)
gf	348.96	kJ/mol	Joback Method
hf	-139.00	kJ/mol	Cheméo Relay (1.0)
hfus	41.50	kJ/mol	Joback Method
hvap	81.61	kJ/mol	Cheméo Relay (1.0)
ie	8.26	eV	Cheméo Relay (1.0)
log10ws	-7.21		Cheméo Relay (1.0)
logp	6.596		Crippen Method
mcvol	251.580	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
tb	568.32	K	Cheméo Relay (1.0)
tc	733.75	K	Cheméo Relay (1.0)
tf	256.48	K	Cheméo Relay (1.0)
vc	0.921	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.23	J/mol×K	616.24	Joback Method
cpg	681.18	J/mol×K	644.76	Joback Method
cpg	699.27	J/mol×K	673.27	Joback Method
cpg	716.53	J/mol×K	701.79	Joback Method
cpg	733.00	J/mol×K	730.30	Joback Method
cpg	748.73	J/mol×K	758.82	Joback Method

cpg	763.77	J/mol×K	787.33	Joback Method
dvisc	0.0036935	Pa×s	280.70	Joback Method
dvisc	0.0012050	Pa×s	336.62	Joback Method
dvisc	0.0005409	Pa×s	392.55	Joback Method
dvisc	0.0002965	Pa×s	448.47	Joback Method
dvisc	0.0001857	Pa×s	504.39	Joback Method
dvisc	0.0001277	Pa×s	560.32	Joback Method
dvisc	0.0000940	Pa×s	616.24	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80625361&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

Legend

af: Acentric Factor
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
ie: Ionization energy
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