Hexadec-11-yn-13,15-diene

Inchi: InChI=1S/C16H26/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h3,5,7H,1,4,6,8,10,12-16H2
InchiKey: FWRSRLMOSLAFAV-FNORWQNLSA-N
Formula: C16H26
SMILES: C=CC=CC#CCCCCCCCCCC
Mol. weight [g/mol]: 218.38

Physical Properties

Property code	Value	Unit	Source
gf	454.70	kJ/mol	Joback Method
hf	141.38	kJ/mol	Joback Method
hfus	39.24	kJ/mol	Joback Method
hvap	52.65	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.263		Crippen Method
mcvol	219.100	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	1626.00		NIST Webbook
rinpol	1626.00		NIST Webbook
tb	575.32	K	Joback Method
tc	759.88	K	Joback Method
tf	369.34	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.65	J/mol×K	575.32	Joback Method
cpg	554.80	J/mol×K	606.08	Joback Method
cpg	572.09	J/mol×K	636.84	Joback Method
cpg	588.56	J/mol×K	667.60	Joback Method
cpg	604.24	J/mol×K	698.36	Joback Method
cpg	619.18	J/mol×K	729.12	Joback Method
cpg	633.40	J/mol×K	759.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R203166&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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