(E,E)-4,8,12-Trimethyl-1,2,7,11-tridecatetraene

Inchi: InChI=1S/C16H26/c1-6-9-15(4)12-8-13-16(5)11-7-10-14(2)3/h9-10,13,15H,1,7-8,11-12H2
InchiKey: NQEIPLKZPFTJNE-DTQAZKPQSA-N
Formula: C16H26
SMILES: C=C=CC(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 218.38

Physical Properties

Property code	Value	Unit	Source
gf	440.86	kJ/mol	Joback Method
hf	124.22	kJ/mol	Joback Method
hfus	32.31	kJ/mol	Joback Method
hvap	50.66	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.436		Crippen Method
mcvol	219.100	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	1582.00		NIST Webbook
tb	573.07	K	Joback Method
tc	763.90	K	Joback Method
tf	221.75	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.51	J/mol×K	573.07	Joback Method
cpg	556.37	J/mol×K	604.87	Joback Method
cpg	574.28	J/mol×K	636.68	Joback Method
cpg	591.30	J/mol×K	668.48	Joback Method
cpg	607.45	J/mol×K	700.29	Joback Method
cpg	622.80	J/mol×K	732.09	Joback Method
cpg	637.37	J/mol×K	763.90	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=R420183&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