(3E,7E)-4,8,12-Trimethyltrideca-1,3,7,11-tetraene

Inchi: InChI=1S/C16H26/c1-6-9-15(4)12-8-13-16(5)11-7-10-14(2)3/h6,9-10,13H,1,7-8,11-12H2,
InchiKey: CWLVBFJCJXHUCF-RNPYNJAESA-N
Formula: C16H26
SMILES: C=CC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 218.38
CAS: 62235-06-7

Physical Properties

Property code	Value	Unit	Source
gf	386.69	kJ/mol	Joback Method
hf	74.15	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	50.65	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.592		Crippen Method
mcvol	219.100	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	1572.90		NIST Webbook
rinpol	1580.90		NIST Webbook
rinpol	1572.90		NIST Webbook
tb	574.28	K	Joback Method
tc	762.61	K	Joback Method
tf	211.20	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.91	J/mol×K	574.28	Joback Method
cpg	553.50	J/mol×K	605.67	Joback Method
cpg	571.11	J/mol×K	637.06	Joback Method
cpg	587.78	J/mol×K	668.44	Joback Method
cpg	603.60	J/mol×K	699.83	Joback Method
cpg	618.61	J/mol×K	731.22	Joback Method

cpg	632.89	J/mol×K	762.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62235067&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
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