1,1,4,8-Tetramethyl-4,7,10-cycloundecatriene

Inchi: InChI=1S/C15H24/c1-13-7-5-8-14(2)10-12-15(3,4)11-6-9-13/h6-8,11H,5,9-10,12H2,1-4H
InchiKey: FVWQAXRELOCFSV-AZDRRDCDSA-N
Formula: C15H24
SMILES: CC1=CCC=C(C)CCC(C)(C)C=CC1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	104.50	kJ/mol	Joback Method
hf	-163.77	kJ/mol	Joback Method
hfus	12.53	kJ/mol	Joback Method
hvap	51.32	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.035		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1472.00		NIST Webbook
tb	591.18	K	Joback Method
tc	827.88	K	Joback Method
tf	299.81	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.93	J/mol×K	591.18	Joback Method
cpg	524.87	J/mol×K	630.63	Joback Method
cpg	547.39	J/mol×K	670.08	Joback Method
cpg	568.60	J/mol×K	709.53	Joback Method
cpg	588.61	J/mol×K	748.98	Joback Method
cpg	607.51	J/mol×K	788.43	Joback Method
cpg	625.41	J/mol×K	827.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R577274&Units=SI

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

Latest version available from:
https://www.chemeo.com/cid/48-579-7/1-1-4-8-Tetramethyl-4-7-10-cycloundecatriene.pdf
Generated by Cheméo on 2024-10-12 03:04:03.361938871 +0000 UTC m=+3283105.998908119.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.