(2Z,4Z,6E)-2,4,6-Undecatriene

Other names: (Z,Z,E)2,4,6-Undecatriene
Inchi: InChI=1S/C11H18/c1-3-5-7-9-11-10-8-6-4-2/h3,5,7,9-11H,4,6,8H2,1-2H3/b5-3+,9-7-,11-1
InchiKey: XQQUSVHISAVPIV-WMSSWCHWSA-N
Formula: C11H18
SMILES: CC=CC=CC=CCCCC
Mol. weight [g/mol]: 150.26
CAS: 85615-64-1

Physical Properties

Property code	Value	Unit	Source
gf	282.40	kJ/mol	Joback Method
hf	81.29	kJ/mol	Joback Method
hfus	24.85	kJ/mol	Joback Method
hvap	39.95	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.865		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1233.00		NIST Webbook
rinpol	1233.00		NIST Webbook
ripol	1470.00		NIST Webbook
tb	463.56	K	Joback Method
tc	648.99	K	Joback Method
tf	198.49	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.95	J/mol×K	463.56	Joback Method
cpg	381.99	J/mol×K	618.09	Joback Method
cpg	369.66	J/mol×K	587.18	Joback Method
cpg	356.65	J/mol×K	556.28	Joback Method
cpg	342.89	J/mol×K	525.37	Joback Method

cpg	328.33	J/mol×K	494.47	Joback Method
cpg	393.66	J/mol×K	648.99	Joback Method
dvisc	0.0001328	Pa×s	463.56	Joback Method
dvisc	0.0001775	Pa×s	419.38	Joback Method
dvisc	0.0002539	Pa×s	375.20	Joback Method
dvisc	0.0003996	Pa×s	331.02	Joback Method
dvisc	0.0007231	Pa×s	286.85	Joback Method
dvisc	0.0016240	Pa×s	242.67	Joback Method
dvisc	0.0052292	Pa×s	198.49	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85615641&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

Legend

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
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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