

5,5,9,9-Tetraethyltridecane

Inchi:	InChI=1S/C21H44/c1-7-13-16-20(9-3,10-4)18-15-19-21(11-5,12-6)17-14-8-2/h7-19H2,1-6
InchiKey:	YRQFTNZUPRLNHZ-UHFFFAOYSA-N
Formula:	C21H44
SMILES:	CCCCC(CC)(CC)CCCC(CC)(CC)CCCC
Mol. weight [g/mol]:	296.57

Physical Properties

Property code	Value	Unit	Source
gf	131.62	kJ/mol	Joback Method
hf	-494.27	kJ/mol	Joback Method
hfus	35.32	kJ/mol	Joback Method
hvap	59.75	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	8.150		Crippen Method
mcvol	306.750	ml/mol	McGowan Method
pc	979.01	kPa	Joback Method
rinpol	1931.00		NIST Webbook
rinpol	1931.00		NIST Webbook
tb	673.42	K	Joback Method
tc	844.37	K	Joback Method
tf	331.27	K	Joback Method
vc	1.190	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.11	J/molxK	673.42	Joback Method
cpg	926.40	J/molxK	701.91	Joback Method
cpg	947.62	J/molxK	730.40	Joback Method
cpg	967.83	J/molxK	758.90	Joback Method
cpg	987.07	J/molxK	787.39	Joback Method
cpg	1005.41	J/molxK	815.88	Joback Method
cpg	1022.90	J/molxK	844.37	Joback Method
dvisc	0.0043469	Paxs	331.27	Joback Method

dvisc	0.0012737	Paxs	388.29	Joback Method
dvisc	0.0005111	Paxs	445.32	Joback Method
dvisc	0.0002523	Paxs	502.34	Joback Method
dvisc	0.0001439	Paxs	559.37	Joback Method
dvisc	0.0000910	Paxs	616.39	Joback Method
dvisc	0.0000622	Paxs	673.42	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=R415453&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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