3,3,11,11-Tetraethyltridecane

Inchi: InChI=1S/C21H44/c1-7-20(8-2,9-3)18-16-14-13-15-17-19-21(10-4,11-5)12-6/h7-19H2,1-6
InchiKey: GVEHWITXYSVWBO-UHFFFAOYSA-N
Formula: C21H44
SMILES: CCC(CC)(CC)CCCCCCCC(CC)(CC)CC
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	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook
tb	673.42	K	Joback Method
tc	844.37	K	Joback Method
tf	331.27	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0012737	Pa×s	388.29	Joback Method
dvisc	0.0005111	Pa×s	445.32	Joback Method
dvisc	0.0002523	Pa×s	502.34	Joback Method
dvisc	0.0001439	Pa×s	559.37	Joback Method
dvisc	0.0000910	Pa×s	616.39	Joback Method
dvisc	0.0000622	Pa×s	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=R415097&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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