

cis-3,6,9,12,15,18-heneicosaene

Inchi:	InChI=1S/C21H32/c1-3-5-7-9-11-13-15-17-19-21-20-18-16-14-12-10-8-6-4-2/h5-8,11-14,
InchiKey:	AMGFAFLDDFGVIQ-YTWBPVBXSA-N
Formula:	C21H32
SMILES:	CCC=CCC=CCC=CCC=CCC=CCC=CCC
Mol. weight [g/mol]:	284.48

Physical Properties

Property code	Value	Unit	Source
gf	607.26	kJ/mol	Joback Method
hf	226.55	kJ/mol	Joback Method
hfus	51.36	kJ/mol	Joback Method
hvap	62.09	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	7.094		Crippen Method
mcvol	280.950	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
rinpol	2004.00		NIST Webbook
ripol	2383.00		NIST Webbook
tb	704.84	K	Joback Method
tc	893.50	K	Joback Method
tf	295.95	K	Joback Method
vc	1.091	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.81	J/mol×K	704.84	Joback Method
cpg	788.59	J/mol×K	736.28	Joback Method
cpg	806.44	J/mol×K	767.73	Joback Method
cpg	823.47	J/mol×K	799.17	Joback Method
cpg	839.78	J/mol×K	830.62	Joback Method
cpg	855.45	J/mol×K	862.06	Joback Method
cpg	870.60	J/mol×K	893.50	Joback Method
dvisc	0.0023871	Paxs	295.95	Joback Method

dvisc	0.0006147	Paxs	364.10	Joback Method
dvisc	0.0002428	Paxs	432.25	Joback Method
dvisc	0.0001235	Paxs	500.39	Joback Method
dvisc	0.0000739	Paxs	568.54	Joback Method
dvisc	0.0000493	Paxs	636.69	Joback Method
dvisc	0.0000356	Paxs	704.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R485680&Units=SI

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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