

Heptadecane, 3,7,11,15-tetramethyl

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C21H44/c1-7-18(3)12-9-14-20(5)16-11-17-21(6)15-10-13-19(4)8-2/h18-21H,7-

HGXQMDBRPYJRTH-UHFFFAOYSA-N

C21H44

CCC(C)CCCC(C)CCCC(C)CCCC(C)CC

296.57

Physical Properties

Property code	Value	Unit	Source
gf	116.18	kJ/mol	Joback Method
hf	-497.89	kJ/mol	Joback Method
hfus	36.05	kJ/mol	Joback Method
hvap	60.79	kJ/mol	Joback Method
log10ws	-7.65		Crippen Method
logp	7.862		Crippen Method
mcvol	306.750	ml/mol	McGowan Method
pc	975.34	kPa	Joback Method
rinpol	1892.00		NIST Webbook
tb	678.12	K	Joback Method
tc	846.24	K	Joback Method
tf	266.43	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.12	J/mol×K	678.12	Joback Method
cpg	924.44	J/mol×K	706.14	Joback Method
cpg	945.77	J/mol×K	734.16	Joback Method
cpg	966.15	J/mol×K	762.18	Joback Method
cpg	985.59	J/mol×K	790.20	Joback Method
cpg	1004.15	J/mol×K	818.22	Joback Method
cpg	1021.83	J/mol×K	846.24	Joback Method
dvisc	0.0164078	Pa×s	266.43	Joback Method
dvisc	0.0025167	Pa×s	335.04	Joback Method

dvisc	0.0007301	Pa×s	403.66	Joback Method
dvisc	0.0003035	Pa×s	472.27	Joback Method
dvisc	0.0001576	Pa×s	540.89	Joback Method
dvisc	0.0000949	Pa×s	609.50	Joback Method
dvisc	0.0000633	Pa×s	678.12	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=R215411&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

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