

5,5-Diethylheptadecane

Inchi:	InChI=1S/C21H44/c1-5-9-11-12-13-14-15-16-17-18-20-21(7-3,8-4)19-10-6-2/h5-20H2,1-4
InchiKey:	VJEBZMJINGAXKO-UHFFFAOYSA-N
Formula:	C21H44
SMILES:	CCCCCCCCCCCCC(CC)(CC)CCCC
Mol. weight [g/mol]:	296.57

Physical Properties

Property code	Value	Unit	Source
gf	128.78	kJ/mol	Joback Method
hf	-485.52	kJ/mol	Joback Method
hfus	42.73	kJ/mol	Joback Method
hvap	61.04	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	8.294		Crippen Method
mcvol	306.750	ml/mol	McGowan Method
pc	967.47	kPa	Joback Method
rinpol	2006.00		NIST Webbook
tb	676.65	K	Joback Method
tc	842.53	K	Joback Method
tf	328.85	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.40	J/mol×K	676.65	Joback Method
cpg	924.16	J/mol×K	704.30	Joback Method
cpg	944.95	J/mol×K	731.94	Joback Method
cpg	964.81	J/mol×K	759.59	Joback Method
cpg	983.77	J/mol×K	787.24	Joback Method
cpg	1001.89	J/mol×K	814.88	Joback Method
cpg	1019.20	J/mol×K	842.53	Joback Method
dvisc	0.0037943	Pa×s	328.85	Joback Method
dvisc	0.0011988	Pa×s	386.82	Joback Method

dvisc	0.0005115	Pa×s	444.78	Joback Method
dvisc	0.0002656	Pa×s	502.75	Joback Method
dvisc	0.0001579	Pa×s	560.72	Joback Method
dvisc	0.0001035	Pa×s	618.68	Joback Method
dvisc	0.0000729	Pa×s	676.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360417&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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