

Hexadecane, 3-heptyl

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C23H48/c1-4-7-9-11-12-13-14-15-16-18-20-22-23(6-3)21-19-17-10-8-5-2/h23H

LHEDVGHANBQGNN-UHFFFAOYSA-N

C23H48

CCCCCCCCCCCCCCC(CC)CCCCCCC

324.63

Physical Properties

Property code	Value	Unit	Source
gf	140.34	kJ/mol	Joback Method
hf	-523.33	kJ/mol	Joback Method
hfus	51.80	kJ/mol	Joback Method
hvap	66.40	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	9.074		Crippen Method
mcvol	334.930	ml/mol	McGowan Method
pc	855.96	kPa	Joback Method
rinpol	2218.00		NIST Webbook
tb	725.20	K	Joback Method
tc	892.42	K	Joback Method
tf	333.97	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.67	J/mol×K	725.20	Joback Method
cpg	1047.11	J/mol×K	753.07	Joback Method
cpg	1068.56	J/mol×K	780.94	Joback Method
cpg	1089.04	J/mol×K	808.81	Joback Method
cpg	1108.60	J/mol×K	836.68	Joback Method
cpg	1127.28	J/mol×K	864.55	Joback Method
cpg	1145.09	J/mol×K	892.42	Joback Method
dvisc	0.0035428	Pa×s	333.97	Joback Method
dvisc	0.0010359	Pa×s	399.17	Joback Method

dvisc	0.0004278	Pa×s	464.38	Joback Method
dvisc	0.0002197	Pa×s	529.59	Joback Method
dvisc	0.0001306	Pa×s	594.79	Joback Method
dvisc	0.0000860	Pa×s	659.99	Joback Method
dvisc	0.0000611	Pa×s	725.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R47625&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

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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