

Hexadecane, 2-heptyl

Other names:	Docosane, 8-methyl
Inchi:	InChI=1S/C23H48/c1-4-6-8-10-11-12-13-14-15-16-18-20-22-23(3)21-19-17-9-7-5-2/h23H
InchiKey:	MGRABISZXSXVCR-UHFFFAOYSA-N
Formula:	C23H48
SMILES:	CCCCCCCCCCCCCCCC(C)CCCCCCC
Mol. weight [g/mol]:	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
mvol	334.930	ml/mol	McGowan Method
pc	855.96	kPa	Joback Method
rinpol	2242.30		NIST Webbook
rinpol	2242.30		NIST Webbook
tb	725.20	K	Joback Method
tc	892.42	K	Joback Method
tf	333.97	K	Joback Method
vc	1.317	m ³ /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	Paxs	333.97	Joback Method
dvisc	0.0010359	Paxs	399.17	Joback Method
dvisc	0.0004278	Paxs	464.38	Joback Method
dvisc	0.0002197	Paxs	529.59	Joback Method
dvisc	0.0001306	Paxs	594.79	Joback Method
dvisc	0.0000860	Paxs	659.99	Joback Method
dvisc	0.0000611	Paxs	725.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R47536&Units=SI
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

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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