

Hexadecane, 7-pentyl-8-propyl

Inchi:	InChI=1S/C24H50/c1-5-9-12-14-15-18-21-23(19-8-4)24(20-16-11-7-3)22-17-13-10-6-2/h
InchiKey:	SXIJAIBMOYCWML-UHFFFAOYSA-N
Formula:	C24H50
SMILES:	CCCCCCCC(CCC)C(CCCCC)CCCCC
Mol. weight [g/mol]:	338.65

Physical Properties

Property code	Value	Unit	Source
gf	146.32	kJ/mol	Joback Method
hf	-549.25	kJ/mol	Joback Method
hfus	50.87	kJ/mol	Joback Method
hvap	68.24	kJ/mol	Joback Method
log10ws	-9.39		Crippen Method
logp	9.320		Crippen Method
mvol	349.020	ml/mol	McGowan Method
pc	813.53	kPa	Joback Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
tb	747.64	K	Joback Method
tc	918.49	K	Joback Method
tf	330.24	K	Joback Method
vc	1.367	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.25	J/molxK	747.64	Joback Method
cpg	1111.28	J/molxK	776.12	Joback Method
cpg	1133.26	J/molxK	804.59	Joback Method
cpg	1154.22	J/molxK	833.07	Joback Method
cpg	1174.19	J/molxK	861.54	Joback Method
cpg	1193.23	J/molxK	890.02	Joback Method
cpg	1211.36	J/molxK	918.49	Joback Method
dvisc	0.0043011	Paxs	330.24	Joback Method

dvisc	0.0010669	Paxs	399.81	Joback Method
dvisc	0.0004001	Paxs	469.37	Joback Method
dvisc	0.0001933	Paxs	538.94	Joback Method
dvisc	0.0001102	Paxs	608.51	Joback Method
dvisc	0.0000706	Paxs	678.07	Joback Method
dvisc	0.0000491	Paxs	747.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R9259&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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