

Hexadecane, 8,9-dibutyl

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C24H50/c1-5-9-13-15-17-21-23(19-11-7-3)24(20-12-8-4)22-18-16-14-10-6-2/h2-4,6-8,10-12,14-16,18-20,22-24H

ZTKGWYHUQJSRJN-UHFFFAOYSA-N

C24H50

CCCCCCCC(CCCC)C(CCCC)CCCCCCC

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
mcvol	349.020	ml/mol	McGowan Method
pc	813.53	kPa	Joback Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
tb	747.64	K	Joback Method
tc	918.49	K	Joback Method
tf	330.24	K	Joback Method
vc	1.367	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0010669	Pa×s	399.81	Joback Method
dvisc	0.0004001	Pa×s	469.37	Joback Method
dvisc	0.0001933	Pa×s	538.94	Joback Method
dvisc	0.0001102	Pa×s	608.51	Joback Method
dvisc	0.0000706	Pa×s	678.07	Joback Method
dvisc	0.0000491	Pa×s	747.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R9262&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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