

3-methyl-heptacosane

Inchi:
InchiKey:
Formula:
SMILES:
Mol. weight [g/mol]:
CAS:

InChI=1S/C28H58/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27

NTRHFQVDDLHZMZ-UHFFFAOYSA-N

C28H58

CCCCCCCCCCCCCCCCCCCCCCCC(C)CC

394.76

14167-66-9

Physical Properties

Property code	Value	Unit	Source
gf	182.44	kJ/mol	Joback Method
hf	-626.53	kJ/mol	Joback Method
hfus	64.75	kJ/mol	Joback Method
hvap	77.53	kJ/mol	Joback Method
log10ws	-11.30		Crippen Method
logp	11.025		Crippen Method
mcvol	405.380	ml/mol	McGowan Method
pc	658.14	kPa	Joback Method
rinpol	2775.00		NIST Webbook
rinpol	2771.00		NIST Webbook
rinpol	2772.00		NIST Webbook
rinpol	2771.60		NIST Webbook
rinpol	2775.00		NIST Webbook
rinpol	2775.00		NIST Webbook
rinpol	2776.10		NIST Webbook
rinpol	2770.00		NIST Webbook
rinpol	2775.00		NIST Webbook
rinpol	2773.00		NIST Webbook
rinpol	2775.00		NIST Webbook
rinpol	2775.00		NIST Webbook
rinpol	2772.00		NIST Webbook
rinpol	2773.00		NIST Webbook
rinpol	2774.00		NIST Webbook
rinpol	2779.00		NIST Webbook
rinpol	2773.00		NIST Webbook
rinpol	2775.00		NIST Webbook
rinpol	2772.00		NIST Webbook
rinpol	2772.00		NIST Webbook

rinpol	2773.00		NIST Webbook
rinpol	2774.00		NIST Webbook
rinpol	2774.00		NIST Webbook
rinpol	2775.00		NIST Webbook
rinpol	2772.00		NIST Webbook
rinpol	2784.00		NIST Webbook
rinpol	2774.00		NIST Webbook
rinpol	2772.00		NIST Webbook
rinpol	2773.00		NIST Webbook
tb	839.60	K	Joback Method
tc	1029.02	K	Joback Method
tf	390.32	K	Joback Method
vc	1.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1348.34	J/mol×K	839.60	Joback Method
cpg	1373.75	J/mol×K	871.17	Joback Method
cpg	1397.85	J/mol×K	902.74	Joback Method
cpg	1420.68	J/mol×K	934.31	Joback Method
cpg	1442.31	J/mol×K	965.88	Joback Method
cpg	1462.81	J/mol×K	997.45	Joback Method
cpg	1482.23	J/mol×K	1029.02	Joback Method
dvisc	0.0017949	Pa×s	390.32	Joback Method
dvisc	0.0005242	Pa×s	465.20	Joback Method
dvisc	0.0002154	Pa×s	540.08	Joback Method
dvisc	0.0001099	Pa×s	614.96	Joback Method
dvisc	0.0000649	Pa×s	689.84	Joback Method
dvisc	0.0000425	Pa×s	764.72	Joback Method
dvisc	0.0000300	Pa×s	839.60	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14167669&Units=SI

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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