

13-Methylheptacosane

Other names:	Heptacosane, 13-methyl
Inchi:	InChI=1S/C28H58/c1-4-6-8-10-12-14-16-17-19-21-23-25-27-28(3)26-24-22-20-18-15-13
InchiKey:	CLFMEEYUFHPNBC-UHFFFAOYSA-N
Formula:	C28H58
SMILES:	CCCCCCCCCCCCCCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]:	394.76
CAS:	15689-72-2

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	2735.00		NIST Webbook
rinpol	2726.00		NIST Webbook
rinpol	2743.00		NIST Webbook
rinpol	2736.00		NIST Webbook
rinpol	2734.00		NIST Webbook
rinpol	2728.00		NIST Webbook
rinpol	2731.00		NIST Webbook
rinpol	2723.30		NIST Webbook
rinpol	2733.00		NIST Webbook
rinpol	2736.00		NIST Webbook
rinpol	2735.00		NIST Webbook
rinpol	2734.00		NIST Webbook
rinpol	2733.00		NIST Webbook
rinpol	2731.00		NIST Webbook
rinpol	2734.00		NIST Webbook
rinpol	2733.00		NIST Webbook
rinpol	2734.00		NIST Webbook
rinpol	2735.00		NIST Webbook
rinpol	2731.00		NIST Webbook

rinpol	2728.00		NIST Webbook
rinpol	2730.00		NIST Webbook
rinpol	2733.00		NIST Webbook
rinpol	2734.00		NIST Webbook
rinpol	2734.00		NIST Webbook
rinpol	2735.00		NIST Webbook
rinpol	2733.00		NIST Webbook
rinpol	2728.00		NIST Webbook
tb	839.60	K	Joback Method
tc	1029.02	K	Joback Method
tf	390.32	K	Joback Method
vc	1.597	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

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=C15689722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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