Octacosane, 13-methyl

Other names: 13-Methyloctacosane
Inchi: InChI=1S/C29H60/c1-4-6-8-10-12-14-16-17-18-20-22-24-26-28-29(3)27-25-23-21-19-15-
InchiKey: LWQCUHJKWNBDGI-UHFFFAOYSA-N
Formula: C29H60
SMILES: CCCCCCCCCCCCCCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]: 408.79

Physical Properties

Property code	Value	Unit	Source
gf	190.86	kJ/mol	Joback Method
hf	-647.17	kJ/mol	Joback Method
hfus	67.34	kJ/mol	Joback Method
hvap	79.76	kJ/mol	Joback Method
log10ws	-11.72		Crippen Method
logp	11.415		Crippen Method
mcvol	419.470	ml/mol	McGowan Method
pc	626.88	kPa	Joback Method
rinpol	2840.00		NIST Webbook
rinpol	2847.00		NIST Webbook
rinpol	2832.00		NIST Webbook
rinpol	2825.00		NIST Webbook
rinpol	2833.00		NIST Webbook
rinpol	2835.00		NIST Webbook
rinpol	2834.60		NIST Webbook
tb	862.48	K	Joback Method
tc	1058.99	K	Joback Method
tf	401.59	K	Joback Method
vc	1.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1415.09	J/mol×K	862.48	Joback Method
cpg	1441.31	J/mol×K	895.23	Joback Method

cpg	1466.11	J/mol×K	927.98	Joback Method
cpg	1489.57	J/mol×K	960.74	Joback Method
cpg	1511.74	J/mol×K	993.49	Joback Method
cpg	1532.71	J/mol×K	1026.24	Joback Method
cpg	1552.54	J/mol×K	1058.99	Joback Method
dvisc	0.0015539	Pa×s	401.59	Joback Method
dvisc	0.0004537	Pa×s	478.40	Joback Method
dvisc	0.0001863	Pa×s	555.22	Joback Method
dvisc	0.0000949	Pa×s	632.04	Joback Method
dvisc	0.0000560	Pa×s	708.85	Joback Method
dvisc	0.0000366	Pa×s	785.66	Joback Method
dvisc	0.0000258	Pa×s	862.48	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=R214067&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