

4-methyloctacosane

Inchi: InChI=1S/C29H60/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29
InchiKey: COKUIQKSCLYMNN-UHFFFAOYSA-N
Formula: C₂₉H₆₀
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCC(C)CCC
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	2864.00		NIST Webbook
rinpol	2856.00		NIST Webbook
rinpol	2860.00		NIST Webbook
rinpol	2859.00		NIST Webbook
rinpol	2855.00		NIST Webbook
rinpol	2853.00		NIST Webbook
rinpol	2858.00		NIST Webbook
rinpol	2859.00		NIST Webbook
rinpol	2865.00		NIST Webbook
rinpol	2860.00		NIST Webbook
rinpol	2860.00		NIST Webbook
tb	862.48	K	Joback Method
tc	1058.99	K	Joback Method
tf	401.59	K	Joback Method
vc	1.653	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1415.09	J/molxK	862.48	Joback Method
cpg	1441.31	J/molxK	895.23	Joback Method
cpg	1466.11	J/molxK	927.98	Joback Method
cpg	1489.57	J/molxK	960.74	Joback Method
cpg	1511.74	J/molxK	993.49	Joback Method
cpg	1532.71	J/molxK	1026.24	Joback Method
cpg	1552.54	J/molxK	1058.99	Joback Method
dvisc	0.0015539	Paxs	401.59	Joback Method
dvisc	0.0004537	Paxs	478.40	Joback Method
dvisc	0.0001863	Paxs	555.22	Joback Method
dvisc	0.0000949	Paxs	632.04	Joback Method
dvisc	0.0000560	Paxs	708.85	Joback Method
dvisc	0.0000366	Paxs	785.66	Joback Method
dvisc	0.0000258	Paxs	862.48	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=R179345&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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