

Heptacosane, 5,17-dimethyl

Inchi:	InChI=1S/C29H60/c1-5-7-9-10-11-15-18-22-26-29(4)27-23-20-17-14-12-13-16-19-21-25
InchiKey:	HNCDSCRIMDABKU-UHFFFAOYSA-N
Formula:	C29H60
SMILES:	CCCCCCCCCCC(C)CCCCCCCCCCCC(C)CCCC
Mol. weight [g/mol]:	408.79

Physical Properties

Property code	Value	Unit	Source
gf	188.42	kJ/mol	Joback Method
hf	-652.45	kJ/mol	Joback Method
hfus	63.82	kJ/mol	Joback Method
hvap	79.37	kJ/mol	Joback Method
log10ws	-11.48		Crippen Method
logp	11.271		Crippen Method
mcvol	419.470	ml/mol	McGowan Method
pc	629.40	kPa	Joback Method
rinpol	2790.00		NIST Webbook
rinpol	2784.00		NIST Webbook
rinpol	2786.00		NIST Webbook
tb	862.04	K	Joback Method
tc	1057.60	K	Joback Method
tf	386.59	K	Joback Method
vc	1.647	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1415.45	J/molxK	862.04	Joback Method
cpg	1441.54	J/molxK	894.63	Joback Method
cpg	1466.21	J/molxK	927.23	Joback Method
cpg	1489.54	J/molxK	959.82	Joback Method
cpg	1511.59	J/molxK	992.41	Joback Method
cpg	1532.42	J/molxK	1025.01	Joback Method
cpg	1552.12	J/molxK	1057.60	Joback Method

dvisc	0.0020179	Paxs	386.59	Joback Method
dvisc	0.0005120	Paxs	465.83	Joback Method
dvisc	0.0001936	Paxs	545.07	Joback Method
dvisc	0.0000937	Paxs	624.31	Joback Method
dvisc	0.0000534	Paxs	703.56	Joback Method
dvisc	0.0000341	Paxs	782.80	Joback Method
dvisc	0.0000236	Paxs	862.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R532840&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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