

Heptacosane, 4-methyl

Inchi:	InChI=1S/C28H58/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-27-2
InchiKey:	GCUWCSFDYYIQEY-UHFFFAOYSA-N
Formula:	C28H58
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCC(C)CCC
Mol. weight [g/mol]:	394.76

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	2760.90		NIST Webbook
rinpol	2760.90		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R570753&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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