

13,25-dimethylhenpentacontane

Inchi:	InChI=1S/C53H108/c1-5-7-9-11-13-15-17-18-19-20-21-22-23-24-25-26-27-28-29-30-33-35
InchiKey:	AFMPPDHZVLGTSO-UHFFFAOYSA-N
Formula:	C53H108
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]:	745.42

Physical Properties

Property code	Value	Unit	Source
gf	390.50	kJ/mol	Joback Method
hf	-1147.81	kJ/mol	Joback Method
hfus	125.98	kJ/mol	Joback Method
hvap	132.80	kJ/mol	Joback Method
log10ws	-21.52		Crippen Method
logp	20.633		Crippen Method
mcvol	757.630	ml/mol	McGowan Method
pc	252.75	kPa	Joback Method
rinpol	5144.00		NIST Webbook
tb	1411.16	K	Joback Method
tc	2468.01	K	Joback Method
tf	657.07	K	Joback Method
vc	2.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3109.86	J/molxK	1411.16	Joback Method
cpg	3221.38	J/molxK	1587.30	Joback Method
cpg	3337.82	J/molxK	1763.44	Joback Method
cpg	3479.47	J/molxK	1939.58	Joback Method
cpg	3666.61	J/molxK	2115.72	Joback Method
cpg	3919.52	J/molxK	2291.87	Joback Method
cpg	4258.48	J/molxK	2468.01	Joback Method
dvisc	0.0000350	Paxs	657.07	Joback Method
dvisc	0.0000094	Paxs	782.75	Joback Method

dvisc	0.0000036	Paxs	908.43	Joback Method
dvisc	0.0000018	Paxs	1034.11	Joback Method
dvisc	0.0000010	Paxs	1159.80	Joback Method
dvisc	0.0000006	Paxs	1285.48	Joback Method
dvisc	0.0000004	Paxs	1411.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R338173&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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