13,23-Dimethylhenpentacontane

Inchi: InChI=1S/C53H108/c1-5-7-9-11-13-15-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-3
InchiKey: BQJVDIBWQPQUKE-UHFFFAOYSA-N
Formula: C53H108
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCC(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
rinpol	5144.00		NIST Webbook
rinpol	5144.00		NIST Webbook
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/mol×K	1411.16	Joback Method
cpg	3221.38	J/mol×K	1587.30	Joback Method
cpg	3337.82	J/mol×K	1763.44	Joback Method
cpg	3479.47	J/mol×K	1939.58	Joback Method
cpg	3666.61	J/mol×K	2115.72	Joback Method
cpg	3919.52	J/mol×K	2291.87	Joback Method

cpg	4258.48	J/mol×K	2468.01	Joback Method
dvisc	0.0000350	Pa×s	657.07	Joback Method
dvisc	0.0000094	Pa×s	782.75	Joback Method
dvisc	0.0000036	Pa×s	908.43	Joback Method
dvisc	0.0000018	Pa×s	1034.11	Joback Method
dvisc	0.0000010	Pa×s	1159.80	Joback Method
dvisc	0.0000006	Pa×s	1285.48	Joback Method
dvisc	0.0000004	Pa×s	1411.16	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R337303&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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