3,9,13,27-tetramethylhentetracontane

Inchi: InChI=1S/C45H92/c1-7-9-10-11-12-13-14-16-19-22-25-29-36-43(4)37-30-26-23-20-17-15
InchiKey: WCVYBNSCGGDIKW-UHFFFAOYSA-N
Formula: C45H92
SMILES: CCCCCCCCCCCCCCC(C)CCCCCCCCCCCCCC(C)CCCC(C)CCCCCC(C)CC
Mol. weight [g/mol]: 633.21

Physical Properties

Property code	Value	Unit	Source
gf	318.26	kJ/mol	Joback Method
hf	-993.25	kJ/mol	Joback Method
hfus	98.21	kJ/mol	Joback Method
hvap	114.21	kJ/mol	Joback Method
log10ws	-17.69		Crippen Method
logp	17.224		Crippen Method
mcvol	644.910	ml/mol	McGowan Method
pc	329.86	kPa	Joback Method
rinpol	4244.00		NIST Webbook
rinpol	4244.00		NIST Webbook
tb	1227.24	K	Joback Method
tc	1732.33	K	Joback Method
tf	536.91	K	Joback Method
vc	2.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2530.47	J/mol×K	1227.24	Joback Method
cpg	2764.94	J/mol×K	1648.15	Joback Method
cpg	2721.40	J/mol×K	1563.97	Joback Method
cpg	2678.06	J/mol×K	1479.78	Joback Method
cpg	2633.03	J/mol×K	1395.60	Joback Method
cpg	2584.46	J/mol×K	1311.42	Joback Method
cpg	2810.54	J/mol×K	1732.33	Joback Method
dvisc	0.0000014	Pa×s	1227.24	Joback Method

dvisc	0.0000021	Pa×s	1112.18	Joback Method
dvisc	0.0000035	Pa×s	997.13	Joback Method
dvisc	0.0000064	Pa×s	882.08	Joback Method
dvisc	0.0000143	Pa×s	767.02	Joback Method
dvisc	0.0000421	Pa×s	651.96	Joback Method
dvisc	0.0001974	Pa×s	536.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R280198&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