

3,9,13,21-tetramethylhentetracontane

Inchi: InChI=1S/C45H92/c1-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-29-36-43(4)37
InchiKey: IYQIUSBGUSTTJ-UHFFFAOYSA-N
Formula: C45H92
SMILES: CCCCCCCCCCCCCCCCCCCCC(C)CCCCCCC(C)CCCC(C)CCCCC(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
tb	1227.24	K	Joback Method
tc	1732.33	K	Joback Method
tf	536.91	K	Joback Method
vc	2.531	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2530.47	J/molxK	1227.24	Joback Method
cpg	2764.94	J/molxK	1648.15	Joback Method
cpg	2721.40	J/molxK	1563.97	Joback Method
cpg	2678.06	J/molxK	1479.78	Joback Method
cpg	2633.03	J/molxK	1395.60	Joback Method
cpg	2584.46	J/molxK	1311.42	Joback Method
cpg	2810.54	J/molxK	1732.33	Joback Method
dvisc	0.0000014	Paxs	1227.24	Joback Method
dvisc	0.0000021	Paxs	1112.18	Joback Method

dvisc	0.0000035	Paxs	997.13	Joback Method
dvisc	0.0000064	Paxs	882.08	Joback Method
dvisc	0.0000143	Paxs	767.02	Joback Method
dvisc	0.0000421	Paxs	651.96	Joback Method
dvisc	0.0001974	Paxs	536.91	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R280183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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