Tetratriacontane, 11-methyl

Inchi: InChI=1S/C45H92/c1-4-6-8-10-12-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30
InchiKey: RGXJUWFUQGQLJC-UHFFFAOYSA-N
Formula: C45H92
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCC
Mol. weight [g/mol]: 633.21

Physical Properties

Property code	Value	Unit	Source
gf	325.58	kJ/mol	Joback Method
hf	-977.41	kJ/mol	Joback Method
hfus	108.78	kJ/mol	Joback Method
hvap	115.38	kJ/mol	Joback Method
log10ws	-18.42		Crippen Method
logp	17.656		Crippen Method
mcvol	644.910	ml/mol	McGowan Method
pc	327.00	kPa	Joback Method
rinpol	3431.00		NIST Webbook
tb	1228.56	K	Joback Method
tc	1771.45	K	Joback Method
tf	581.91	K	Joback Method
vc	2.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2531.87	J/mol×K	1228.56	Joback Method
cpg	2590.82	J/mol×K	1319.04	Joback Method
cpg	2643.96	J/mol×K	1409.52	Joback Method
cpg	2693.62	J/mol×K	1500.00	Joback Method
cpg	2742.13	J/mol×K	1590.48	Joback Method
cpg	2791.82	J/mol×K	1680.97	Joback Method
cpg	2845.01	J/mol×K	1771.45	Joback Method
dvisc	0.0001234	Pa×s	581.91	Joback Method
dvisc	0.0000360	Pa×s	689.68	Joback Method

dvisc	0.0000147	Pa×s	797.46	Joback Method
dvisc	0.0000074	Pa×s	905.23	Joback Method
dvisc	0.0000043	Pa×s	1013.01	Joback Method
dvisc	0.0000028	Pa×s	1120.78	Joback Method
dvisc	0.0000019	Pa×s	1228.56	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=R584628&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