

Tetratriacontane, 12-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: ZWGXCNLMUDAZTQ-UHFFFAOYSA-N
Formula: C45H92
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCC
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
mvol	644.910	ml/mol	McGowan Method
pc	327.00	kPa	Joback Method
rinpol	3431.00		NIST Webbook
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2531.87	J/molxK	1228.56	Joback Method
cpg	2791.82	J/molxK	1680.97	Joback Method
cpg	2742.13	J/molxK	1590.48	Joback Method
cpg	2693.62	J/molxK	1500.00	Joback Method
cpg	2643.96	J/molxK	1409.52	Joback Method
cpg	2590.82	J/molxK	1319.04	Joback Method
cpg	2845.01	J/molxK	1771.45	Joback Method
dvisc	0.0000019	Paxs	1228.56	Joback Method

dvisc	0.0000028	Paxs	1120.78	Joback Method
dvisc	0.0000043	Paxs	1013.01	Joback Method
dvisc	0.0000074	Paxs	905.23	Joback Method
dvisc	0.0000147	Paxs	797.46	Joback Method
dvisc	0.0000360	Paxs	689.68	Joback Method
dvisc	0.0001234	Paxs	581.91	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R584648&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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