

7,11,19-trimethylhentetracontane

Inchi: InChI=1S/C44H90/c1-6-8-10-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-28-32-37-44
InchiKey: KQVZSJLBPALTFP-UHFFFAOYSA-N
Formula: C44H90
SMILES: CCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCC(C)CCCC(C)CCCCC
Mol. weight [g/mol]: 619.19

Physical Properties

Property code	Value	Unit	Source
gf	312.28	kJ/mol	Joback Method
hf	-967.33	kJ/mol	Joback Method
hfus	99.15	kJ/mol	Joback Method
hvap	112.37	kJ/mol	Joback Method
log10ws	-17.52		Crippen Method
logp	16.978		Crippen Method
mcvol	630.820	ml/mol	McGowan Method
pc	340.66	kPa	Joback Method
rinpol	4177.00		NIST Webbook
tb	1204.80	K	Joback Method
tc	1682.83	K	Joback Method
tf	540.64	K	Joback Method
vc	2.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2459.60	J/molxK	1204.80	Joback Method
cpg	2511.69	J/molxK	1284.47	Joback Method
cpg	2558.56	J/molxK	1364.14	Joback Method
cpg	2601.77	J/molxK	1443.82	Joback Method
cpg	2642.87	J/molxK	1523.49	Joback Method
cpg	2683.40	J/molxK	1603.16	Joback Method
cpg	2724.92	J/molxK	1682.83	Joback Method
dvisc	0.0001986	Paxs	540.64	Joback Method
dvisc	0.0000473	Paxs	651.33	Joback Method

dvisc	0.0000171	Paxs	762.03	Joback Method
dvisc	0.0000080	Paxs	872.72	Joback Method
dvisc	0.0000044	Paxs	983.41	Joback Method
dvisc	0.0000028	Paxs	1094.11	Joback Method
dvisc	0.0000019	Paxs	1204.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R280549&Units=SI

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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