

16,20,24-Trimethyloctartiacontane

Inchi:	InChI=1S/C41H84/c1-6-8-10-12-14-16-18-20-22-24-26-28-30-34-40(4)36-32-38-41(5)37-
InchiKey:	BSLLKNWCRUBRDR-UHFFFAOYSA-N
Formula:	C41H84
SMILES:	CCCCCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCC
Mol. weight [g/mol]:	577.11

Physical Properties

Property code	Value	Unit	Source
gf	287.02	kJ/mol	Joback Method
hf	-905.41	kJ/mol	Joback Method
hfus	91.38	kJ/mol	Joback Method
hvap	105.70	kJ/mol	Joback Method
log10ws	-16.26		Crippen Method
logp	15.808		Crippen Method
mcvol	588.550	ml/mol	McGowan Method
pc	379.98	kPa	Joback Method
rinpol	3784.00		NIST Webbook
rinpol	3784.00		NIST Webbook
rinpol	3874.00		NIST Webbook
tb	1136.16	K	Joback Method
tc	1517.43	K	Joback Method
tf	506.83	K	Joback Method
vc	2.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2246.59	J/molxK	1136.16	Joback Method
cpg	2290.12	J/molxK	1199.71	Joback Method
cpg	2329.56	J/molxK	1263.25	Joback Method
cpg	2365.64	J/molxK	1326.80	Joback Method
cpg	2399.11	J/molxK	1390.34	Joback Method
cpg	2430.68	J/molxK	1453.89	Joback Method
cpg	2461.09	J/molxK	1517.43	Joback Method

dvisc	0.0003383	Paxs	506.83	Joback Method
dvisc	0.0000794	Paxs	611.72	Joback Method
dvisc	0.0000285	Paxs	716.61	Joback Method
dvisc	0.0000133	Paxs	821.49	Joback Method
dvisc	0.0000074	Paxs	926.38	Joback Method
dvisc	0.0000046	Paxs	1031.27	Joback Method
dvisc	0.0000031	Paxs	1136.16	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=R505185&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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