

5,13,17-Trimethylheptartiacontane

Inchi: InChI=1S/C40H82/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-28-34-39(4)30
InchiKey: QXQCNUFHHTHTDL-UHFFFAOYSA-N
Formula: C40H82
SMILES: CCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCC(C)CCCC
Mol. weight [g/mol]: 563.08

Physical Properties

Property code	Value	Unit	Source
gf	278.60	kJ/mol	Joback Method
hf	-884.77	kJ/mol	Joback Method
hfus	88.79	kJ/mol	Joback Method
hvap	103.47	kJ/mol	Joback Method
log10ws	-15.84		Crippen Method
logp	15.418		Crippen Method
mcvol	574.460	ml/mol	McGowan Method
pc	394.61	kPa	Joback Method
rinpol	3803.00		NIST Webbook
rinpol	3803.00		NIST Webbook
rinpol	3803.00		NIST Webbook
tb	1113.28	K	Joback Method
tc	1468.24	K	Joback Method
tf	495.56	K	Joback Method
vc	2.257	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2175.93	J/molxK	1113.28	Joback Method
cpg	2217.11	J/molxK	1172.44	Joback Method
cpg	2254.57	J/molxK	1231.60	Joback Method
cpg	2288.88	J/molxK	1290.76	Joback Method
cpg	2320.61	J/molxK	1349.92	Joback Method
cpg	2350.35	J/molxK	1409.08	Joback Method
cpg	2378.66	J/molxK	1468.24	Joback Method

dvisc	0.0004037	Paxs	495.56	Joback Method
dvisc	0.0000943	Paxs	598.51	Joback Method
dvisc	0.0000337	Paxs	701.47	Joback Method
dvisc	0.0000157	Paxs	804.42	Joback Method
dvisc	0.0000087	Paxs	907.37	Joback Method
dvisc	0.0000054	Paxs	1010.33	Joback Method
dvisc	0.0000037	Paxs	1113.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R505501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mvol:	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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