3,7,15-trimethyl-heptatriacontane

Inchi: InChI=1S/C40H82/c1-6-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-26-29-33-39
InchiKey: JOINQOCWDNVBSJ-UHFFFAOYSA-N
Formula: C40H82
SMILES: CCCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCC(C)CCCC(C)CC
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	3835.00		NIST Webbook
rinpol	3837.00		NIST Webbook
rinpol	3837.00		NIST Webbook
rinpol	3835.00		NIST Webbook
rinpol	3835.00		NIST Webbook
tb	1113.28	K	Joback Method
tc	1468.24	K	Joback Method
tf	495.56	K	Joback Method
vc	2.257	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2175.93	J/mol×K	1113.28	Joback Method
cpg	2350.35	J/mol×K	1409.08	Joback Method
cpg	2320.61	J/mol×K	1349.92	Joback Method
cpg	2288.88	J/mol×K	1290.76	Joback Method
cpg	2254.57	J/mol×K	1231.60	Joback Method

cpg	2217.11	J/mol×K	1172.44	Joback Method
cpg	2378.66	J/mol×K	1468.24	Joback Method
dvisc	0.0000037	Pa×s	1113.28	Joback Method
dvisc	0.0000054	Pa×s	1010.33	Joback Method
dvisc	0.0000087	Pa×s	907.37	Joback Method
dvisc	0.0000157	Pa×s	804.42	Joback Method
dvisc	0.0000337	Pa×s	701.47	Joback Method
dvisc	0.0000943	Pa×s	598.51	Joback Method
dvisc	0.0004037	Pa×s	495.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R272345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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