

13,17,21-Trimethylpentatriacontane

Inchi:	InChI=1S/C38H78/c1-6-8-10-12-14-16-18-19-21-23-25-27-31-37(4)33-29-35-38(5)34-28
InchiKey:	WWWYYEDTJKBCOF-UHFFFAOYSA-N
Formula:	C38H78
SMILES:	CCCCCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]:	535.03
CAS:	58668-39-6

Physical Properties

Property code	Value	Unit	Source
gf	261.76	kJ/mol	Joback Method
hf	-843.49	kJ/mol	Joback Method
hfus	83.61	kJ/mol	Joback Method
hvap	99.02	kJ/mol	Joback Method
log10ws	-15.00		Crippen Method
logp	14.637		Crippen Method
mcvol	546.280	ml/mol	McGowan Method
pc	426.53	kPa	Joback Method
rinpol	3577.00		NIST Webbook
rinpol	3580.00		NIST Webbook
rinpol	3580.00		NIST Webbook
rinpol	3577.00		NIST Webbook
rinpol	3582.00		NIST Webbook
tb	1067.52	K	Joback Method
tc	1377.25	K	Joback Method
tf	473.02	K	Joback Method
vc	2.146	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2035.18	J/molxK	1067.52	Joback Method
cpg	2072.28	J/molxK	1119.14	Joback Method
cpg	2106.31	J/molxK	1170.76	Joback Method
cpg	2137.62	J/molxK	1222.39	Joback Method

cpg	2166.59	J/mol×K	1274.01	Joback Method
cpg	2193.56	J/mol×K	1325.63	Joback Method
cpg	2218.90	J/mol×K	1377.25	Joback Method
dvisc	0.0005738	Paxs	473.02	Joback Method
dvisc	0.0001326	Paxs	572.10	Joback Method
dvisc	0.0000472	Paxs	671.19	Joback Method
dvisc	0.0000219	Paxs	770.27	Joback Method
dvisc	0.0000121	Paxs	869.35	Joback Method
dvisc	0.0000076	Paxs	968.44	Joback Method
dvisc	0.0000052	Paxs	1067.52	Joback Method

Sources

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=C58668396&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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