

12,16,20-Trimethyltetratriacontane

Inchi:	InChI=1S/C37H76/c1-6-8-10-12-14-16-17-18-20-22-24-26-30-36(4)32-28-34-37(5)33-27-
InchiKey:	ICWKHVKXWKXSHR-UHFFFAOYSA-N
Formula:	C37H76
SMILES:	CCCCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]:	521.00

Physical Properties

Property code	Value	Unit	Source
gf	253.34	kJ/mol	Joback Method
hf	-822.85	kJ/mol	Joback Method
hfus	81.02	kJ/mol	Joback Method
hvap	96.79	kJ/mol	Joback Method
log10ws	-14.59		Crippen Method
logp	14.247		Crippen Method
mcvol	532.190	ml/mol	McGowan Method
pc	443.96	kPa	Joback Method
rinpol	3478.00		NIST Webbook
rinpol	3484.00		NIST Webbook
rinpol	3478.00		NIST Webbook
rinpol	3478.00		NIST Webbook
tb	1044.64	K	Joback Method
tc	1335.05	K	Joback Method
tf	461.75	K	Joback Method
vc	2.090	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1965.12	J/molxK	1044.64	Joback Method
cpg	2000.46	J/molxK	1093.04	Joback Method
cpg	2032.99	J/molxK	1141.44	Joback Method
cpg	2063.03	J/molxK	1189.85	Joback Method
cpg	2090.85	J/molxK	1238.25	Joback Method
cpg	2116.75	J/molxK	1286.65	Joback Method

cpg	2141.02	J/mol×K	1335.05	Joback Method
dvisc	0.0006836	Paxs	461.75	Joback Method
dvisc	0.0001570	Paxs	558.90	Joback Method
dvisc	0.0000558	Paxs	656.05	Joback Method
dvisc	0.0000259	Paxs	753.19	Joback Method
dvisc	0.0000143	Paxs	850.34	Joback Method
dvisc	0.0000089	Paxs	947.49	Joback Method
dvisc	0.0000061	Paxs	1044.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R505130&Units=SI
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

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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