2,12,20-Trimethyltriacontane

Inchi: InChI=1S/C33H68/c1-6-7-8-9-10-13-17-22-27-32(4)29-24-19-15-20-25-30-33(5)28-23-18
InchiKey: NDUCMLJZRHJPPD-UHFFFAOYSA-N
Formula: C33H68
SMILES: CCCCCCCCCCC(C)CCCCCCCC(C)CCCCCCCCCC(C)C
Mol. weight [g/mol]: 464.89

Physical Properties

Property code	Value	Unit	Source
gf	219.66	kJ/mol	Joback Method
hf	-740.29	kJ/mol	Joback Method
hfus	70.66	kJ/mol	Joback Method
hvap	87.89	kJ/mol	Joback Method
log10ws	-12.91		Crippen Method
logp	12.687		Crippen Method
mcvol	475.830	ml/mol	McGowan Method
pc	525.57	kPa	Joback Method
rinpol	3123.00		NIST Webbook
rinpol	3123.00		NIST Webbook
tb	953.12	K	Joback Method
tc	1184.34	K	Joback Method
tf	416.67	K	Joback Method
vc	1.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1687.56	J/mol×K	953.12	Joback Method
cpg	1717.27	J/mol×K	991.66	Joback Method
cpg	1745.05	J/mol×K	1030.19	Joback Method
cpg	1771.03	J/mol×K	1068.73	Joback Method
cpg	1795.33	J/mol×K	1107.26	Joback Method
cpg	1818.10	J/mol×K	1145.80	Joback Method
cpg	1839.46	J/mol×K	1184.34	Joback Method
dvisc	0.0013680	Pa×s	416.67	Joback Method

dvisc	0.0003061	Pa×s	506.08	Joback Method
dvisc	0.0001074	Pa×s	595.49	Joback Method
dvisc	0.0000495	Pa×s	684.89	Joback Method
dvisc	0.0000273	Pa×s	774.30	Joback Method
dvisc	0.0000170	Pa×s	863.71	Joback Method
dvisc	0.0000116	Pa×s	953.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R337789&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
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
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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