

9,13,20-Trimethyldotriacontane

Inchi: InChI=1S/C35H72/c1-6-8-10-12-14-15-16-17-19-23-27-33(3)28-24-20-21-25-30-35(5)32-34
InchiKey: MLQIOOHLVRFELT-UHFFFAOYSA-N
Formula: C35H72
SMILES: CCCCCCCCCCCCC(C)CCCCCCC(C)CCCC(C)CCCCCCCCC
Mol. weight [g/mol]: 492.95

Physical Properties

Property code	Value	Unit	Source
gf	236.50	kJ/mol	Joback Method
hf	-781.57	kJ/mol	Joback Method
hfus	75.84	kJ/mol	Joback Method
hvap	92.34	kJ/mol	Joback Method
log10ws	-13.75		Crippen Method
logp	13.467		Crippen Method
mcvol	504.010	ml/mol	McGowan Method
pc	482.19	kPa	Joback Method
rinpol	3363.00		NIST Webbook
tb	998.88	K	Joback Method
tc	1256.37	K	Joback Method
tf	439.21	K	Joback Method
vc	1.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1825.75	J/mol×K	998.88	Joback Method
cpg	1858.01	J/mol×K	1041.80	Joback Method
cpg	1887.94	J/mol×K	1084.71	Joback Method
cpg	1915.76	J/mol×K	1127.63	Joback Method
cpg	1941.65	J/mol×K	1170.54	Joback Method
cpg	1965.80	J/mol×K	1213.46	Joback Method
cpg	1988.40	J/mol×K	1256.37	Joback Method
dvisc	0.0009683	Pa×s	439.21	Joback Method
dvisc	0.0002197	Pa×s	532.49	Joback Method

dvisc	0.0000775	Pa×s	625.77	Joback Method
dvisc	0.0000359	Pa×s	719.05	Joback Method
dvisc	0.0000198	Pa×s	812.32	Joback Method
dvisc	0.0000124	Pa×s	905.60	Joback Method
dvisc	0.0000084	Pa×s	998.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R525827&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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