

3,7,11-trimethyl-nonacosane

Inchi:	InChI=1S/C32H66/c1-6-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-31(4)28-24-29
InchiKey:	GQQCWHAYEUVG0I-UHFFFAOYSA-N
Formula:	C32H66
SMILES:	CCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CC
Mol. weight [g/mol]:	450.87

Physical Properties

Property code	Value	Unit	Source
gf	211.24	kJ/mol	Joback Method
hf	-719.65	kJ/mol	Joback Method
hfus	68.07	kJ/mol	Joback Method
hvap	85.66	kJ/mol	Joback Method
log10ws	-12.49		Crippen Method
logp	12.297		Crippen Method
mcvol	461.740	ml/mol	McGowan Method
pc	549.49	kPa	Joback Method
rinpol	3037.00		NIST Webbook
rinpol	3037.00		NIST Webbook
rinpol	3037.00		NIST Webbook
rinpol	3037.00		NIST Webbook
tb	930.24	K	Joback Method
tc	1150.49	K	Joback Method
tf	405.40	K	Joback Method
vc	1.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1618.98	J/molxK	930.24	Joback Method
cpg	1647.60	J/molxK	966.95	Joback Method
cpg	1674.45	J/molxK	1003.66	Joback Method
cpg	1699.63	J/molxK	1040.36	Joback Method
cpg	1723.25	J/molxK	1077.07	Joback Method
cpg	1745.43	J/molxK	1113.78	Joback Method

cpg	1766.27	J/mol×K	1150.49	Joback Method
dvisc	0.0016243	Paxs	405.40	Joback Method
dvisc	0.0003607	Paxs	492.87	Joback Method
dvisc	0.0001261	Paxs	580.35	Joback Method
dvisc	0.0000581	Paxs	667.82	Joback Method
dvisc	0.0000320	Paxs	755.29	Joback Method
dvisc	0.0000199	Paxs	842.77	Joback Method
dvisc	0.0000136	Paxs	930.24	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R300351&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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