13,21,25-trimethyl-nonatriacontane

Inchi: InChI=1S/C42H86/c1-6-8-10-12-14-16-18-19-21-23-26-30-36-41(4)38-33-39-42(5)37-32-
InchiKey: NOGRSPRNENYZMU-UHFFFAOYSA-N
Formula: C42H86
SMILES: CCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]: 591.13

Physical Properties

Property code	Value	Unit	Source
gf	295.44	kJ/mol	Joback Method
hf	-926.05	kJ/mol	Joback Method
hfus	93.97	kJ/mol	Joback Method
hvap	107.92	kJ/mol	Joback Method
log10ws	-16.68		Crippen Method
logp	16.198		Crippen Method
mcvol	602.640	ml/mol	McGowan Method
pc	366.15	kPa	Joback Method
rinpol	3980.00		NIST Webbook
rinpol	3980.00		NIST Webbook
rinpol	3980.00		NIST Webbook
tb	1159.04	K	Joback Method
tc	1569.41	K	Joback Method
tf	518.10	K	Joback Method
vc	2.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2317.43	J/mol×K	1159.04	Joback Method
cpg	2363.53	J/mol×K	1227.44	Joback Method
cpg	2405.17	J/mol×K	1295.83	Joback Method
cpg	2443.29	J/mol×K	1364.23	Joback Method
cpg	2478.81	J/mol×K	1432.62	Joback Method
cpg	2512.67	J/mol×K	1501.02	Joback Method
cpg	2545.81	J/mol×K	1569.41	Joback Method

dvisc	0.0002834	Pa×s	518.10	Joback Method
dvisc	0.0000668	Pa×s	624.92	Joback Method
dvisc	0.0000240	Pa×s	731.75	Joback Method
dvisc	0.0000112	Pa×s	838.57	Joback Method
dvisc	0.0000062	Pa×s	945.39	Joback Method
dvisc	0.0000039	Pa×s	1052.22	Joback Method
dvisc	0.0000026	Pa×s	1159.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R272078&Units=SI

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