13,17,21-TRIMETHYLTRITRIACONTANE

Inchi: InChI=1S/C36H74/c1-6-8-10-12-14-16-18-20-22-24-28-34(3)30-26-32-36(5)33-27-31-35(
InchiKey: VPNSAYIYZOPVGL-UHFFFAOYSA-N
Formula: C36H74
SMILES: CCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]: 506.99

Physical Properties

Property code	Value	Unit	Source
af	1.2924		Cheméo Relay (1.0)
gf	244.92	kJ/mol	Joback Method
hf	-843.67	kJ/mol	Cheméo Relay (1.0)
hfus	78.43	kJ/mol	Joback Method
hvap	160.68	kJ/mol	Cheméo Relay (1.0)
ie	10.05	eV	Cheméo Relay (1.0)
log10ws	-12.77		Cheméo Relay (1.0)
logp	13.857		Crippen Method
mcvol	518.100	ml/mol	McGowan Method
pc	462.48	kPa	Joback Method
rinpol	3375.00		NIST Webbook
rinpol	3377.00		NIST Webbook
rinpol	3379.00		NIST Webbook
tb	679.83	K	Cheméo Relay (1.0)
tc	846.29	K	Cheméo Relay (1.0)
tf	278.31	K	Cheméo Relay (1.0)
vc	2.005	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1895.31	J/mol×K	1021.76	Joback Method
cpg	1929.03	J/mol×K	1067.27	Joback Method
cpg	1960.20	J/mol×K	1112.78	Joback Method
cpg	1989.08	J/mol×K	1158.29	Joback Method
cpg	2015.88	J/mol×K	1203.80	Joback Method

cpg	2040.85	J/mol×K	1249.30	Joback Method
cpg	2064.22	J/mol×K	1294.81	Joback Method
dvisc	0.0008138	Pa×s	450.48	Joback Method
dvisc	0.0001858	Pa×s	545.69	Joback Method
dvisc	0.0000658	Pa×s	640.91	Joback Method
dvisc	0.0000305	Pa×s	736.12	Joback Method
dvisc	0.0000168	Pa×s	831.33	Joback Method
dvisc	0.0000105	Pa×s	926.55	Joback Method
dvisc	0.0000072	Pa×s	1021.76	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58668385&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
ie: Ionization energy
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