3-Methyldotriacontane

Inchi: InChI=1S/C33H68/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-2
InchiKey: YXJZLSDRPAJSLL-UHFFFAOYSA-N
Formula: C33H68
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CC
Mol. weight [g/mol]: 464.91

Physical Properties

Property code	Value	Unit	Source
af	1.2766		Cheméo Relay (1.0)
gf	224.54	kJ/mol	Joback Method
hf	-741.17	kJ/mol	Cheméo Relay (1.0)
hfus	77.70	kJ/mol	Joback Method
hvap	161.44	kJ/mol	Cheméo Relay (1.0)
ie	10.25	eV	Cheméo Relay (1.0)
log10ws	-12.11		Cheméo Relay (1.0)
logp	12.975		Crippen Method
mcvol	475.830	ml/mol	McGowan Method
pc	521.73	kPa	Joback Method
rinpol	3278.00		NIST Webbook
rinpol	3274.00		NIST Webbook
rinpol	3273.40		NIST Webbook
rinpol	3275.00		NIST Webbook
rinpol	3275.00		NIST Webbook
rinpol	3279.00		NIST Webbook
tb	658.92	K	Cheméo Relay (1.0)
tc	828.41	K	Cheméo Relay (1.0)
tf	316.32	K	Cheméo Relay (1.0)
vc	1.877	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1687.02	J/mol×K	954.00	Joback Method
cpg	1717.48	J/mol×K	993.41	Joback Method

cpg	1745.95	J/mol×K	1032.83	Joback Method
cpg	1772.57	J/mol×K	1072.24	Joback Method
cpg	1797.49	J/mol×K	1111.65	Joback Method
cpg	1820.84	J/mol×K	1151.07	Joback Method
cpg	1842.77	J/mol×K	1190.48	Joback Method
dvisc	0.0008545	Pa×s	446.67	Joback Method
dvisc	0.0002494	Pa×s	531.22	Joback Method
dvisc	0.0001021	Pa×s	615.78	Joback Method
dvisc	0.0000519	Pa×s	700.34	Joback Method
dvisc	0.0000305	Pa×s	784.89	Joback Method
dvisc	0.0000199	Pa×s	869.44	Joback Method
dvisc	0.0000140	Pa×s	954.00	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20129491&Units=SI

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