13-Methyldotriacontane

Inchi: InChI=1S/C33H68/c1-4-6-8-10-12-14-16-17-18-19-20-21-22-24-26-28-30-32-33(3)31-29-
InchiKey: KDIOBJDKGGLUPU-UHFFFAOYSA-N
Formula: C33H68
SMILES: CCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCC
Mol. weight [g/mol]: 464.89

Physical Properties

Property code	Value	Unit	Source
gf	224.54	kJ/mol	Joback Method
hf	-729.73	kJ/mol	Joback Method
hfus	77.70	kJ/mol	Joback Method
hvap	88.66	kJ/mol	Joback Method
log10ws	-13.39		Crippen Method
logp	12.975		Crippen Method
mcvol	475.830	ml/mol	McGowan Method
pc	521.73	kPa	Joback Method
rinpol	3232.00		NIST Webbook
rinpol	3235.00		NIST Webbook
rinpol	3238.00		NIST Webbook
rinpol	3228.00		NIST Webbook
rinpol	3227.00		NIST Webbook
tb	954.00	K	Joback Method
tc	1190.48	K	Joback Method
tf	446.67	K	Joback Method
vc	1.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1687.02	J/mol×K	954.00	Joback Method
cpg	1820.84	J/mol×K	1151.07	Joback Method
cpg	1797.49	J/mol×K	1111.65	Joback Method
cpg	1772.57	J/mol×K	1072.24	Joback Method
cpg	1745.95	J/mol×K	1032.83	Joback Method

cpg	1717.48	J/mol×K	993.41	Joback Method
cpg	1842.77	J/mol×K	1190.48	Joback Method
dvisc	0.0000140	Pa×s	954.00	Joback Method
dvisc	0.0000199	Pa×s	869.44	Joback Method
dvisc	0.0000305	Pa×s	784.89	Joback Method
dvisc	0.0000519	Pa×s	700.34	Joback Method
dvisc	0.0001021	Pa×s	615.78	Joback Method
dvisc	0.0002494	Pa×s	531.22	Joback Method
dvisc	0.0008545	Pa×s	446.67	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=R272127&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