2-Methyldotriacontane

Other names: Dotriacontane, 2-methyl
Inchi: InChI=1S/C33H68/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26
InchiKey: ZMRQKNNNZMSHKH-UHFFFAOYSA-N
Formula: C33H68
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 464.89
CAS: 1720-11-2

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	3264.00		NIST Webbook
rinpol	3262.00		NIST Webbook
rinpol	3259.90		NIST Webbook
rinpol	3262.00		NIST Webbook
rinpol	3254.00		NIST Webbook
rinpol	3254.00		NIST Webbook
rinpol	3259.90		NIST Webbook
rinpol	3264.00		NIST Webbook
rinpol	3263.00		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	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
hvapt	122.90	kJ/mol	611.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1720112&Units=SI
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

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
hvapt: Enthalpy of vaporization at a given temperature
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